BIBLIOGRAPHIC DATA SHEET

1. Report No. APTD-1138

2.

PB 211 058

4. Title and Subtitle

A Theoretical Study of NO_x Absorption Using Aqueous Alkaline and Dry Sorbents Volume II

5. Report Date 31 December 1971

6.

7. Author(s)

8. Performing Organization Rept. No. RAD-71-200-007-01

9. Performing Organization Name and Address

RADIAN CORPORATION
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P. O. Box 9948
Austin, Texas 78757

10. Project/Task/Work Unit No.

11. Contract/Grant No. EHSD 71-5

12. Sponsoring Organization Name and Address

Office of Air Programs
ENVIRONMENTAL PROTECTION AGENCY
411 West Chapel Hill Street
Durham, North Carolina 27701

13. Type of Report & Period Covered Final

14.

15. Supplementary Notes

16. Abstracts

Technical notes pertaining to, and developed during, a study of the theoretical description of aqueous scrubbing processes for NO_x emission control are presented. The ten notes are as follows: (1)Review of the literature on experimental studies of the aqueous absorption of nitrogen oxides, (2) Gas phase equilibrium in the system NO_x-H_2O, (3) Compilation of thermodynamic properties for compounds of interest in nitrogen oxides aqueous absorption processes, (4) High temperature behavior of anhydrous and hydrated nitrites and nitrates, (5) Material balance calculations for NO_x aqueous sorption in a packed tower, (6) Selected values for equilibrium constants used in the aqueous equilibrium formulation, (7) Vapor film mass transfer coefficients for HNO_2 and HNO_3 in a packed tower, (8) Results of literature search on aqueous sorption of nitrogen oxides, (9) Calculation of decomposition pressures over metal nitrates and nitrites and, (10) Listing of subroutines for the gas phase equilibrium model.

17. Key Words and Document Analysis. 17a. Descriptors

Air pollution
Nitrogen oxides
Absorptivity
Absorbers
Gas dynamics
Thermodynamic properties
High temperature tests
Sorption

17b. Identifiers/Open-Ended Terms

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NATIONAL TECHNICAL
INFORMATION SERVICE
U S Department of Commerce
Springfield VA 22151

17c. COSATI Field/Group 13B, 7D

18. Availability Statement

Unlimited

19. Security Class (This Report) UNCLASSIFIED

20. Security Class (This Page UNCLASSIFIED

21. No. of Pages 303

22. Price 6 00

R

1a

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RAD-71-200-007-01

FINAL REPORT
VOLUME II

OAP Contract No. EHSD 71-5

A THEORETICAL STUDY OF NO_x ABSORPTION USING AQUEOUS ALKALINE AND DRY SORBENTS

Presented to:

OFFICE OF AIR PROGRAMS
ENVIRONMENTAL PROTECTION AGENCY
411 West Chapel Hill Street
Durham, North Caroline 27701

31 December 1971

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LIST OF TECHNICAL NOTES
IN VOLUME II

Technical Note Number	Title
200-007-02	Review of the Literature on Experimental Studies of the Aqueous Absorption of Nitrogen Oxides
200-007-03a	Gas Phase Equilibrium in the System NO_x - H_2O
200-007-04a	Compilation of Thermodynamic Properties for Compounds of Interest in Nitrogen Oxides Aqueous Absorption Processes
200-007-06	High Temperature Behavior of Anhydrous and Hydrated Nitrites and Nitrates
200-007-09	Material Balance Calculations for NO_x Aqueous Sorption in a Packed Tower
200-007-11	Selected Values for Equilibrium Constants Used in the Aqueous Equilibrium Formulation
200-007-12	Vapor Film Mass Transfer Coefficients for HNO_2 and HNO_3 in a Packed Tower
200-007-14	Results of Literature Search on Aqueous Sorption of Nitrogen Oxides
200-007-15	Calculation of Decomposition Pressures Over Metal Nitrates and Nitrites
200-007-16	Listing of Subroutines for the Gas Phase Equilibrium Model

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TECHNICAL NOTE 200-007-02

REVIEW OF THE LITERATURE ON EXPERIMENTAL STUDIES OF THE AQUEOUS ABSORPTION OF NITROGEN OXIDES

8 January 1971

Prepared by:

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CHEMICAL RESEARCH • SYSTEMS ANALYSIS • COMPUTER SCIENCE • CHEMICAL ENGINEERING

1.0 INTRODUCTION

From the literature search to find information for a theoretical description of sorption processes, it was found that much had been published concerning experimental studies of the rate and mechanism of aqueous sorption of nitrogen oxides. A review of the results that had been previously reported was considered an essential first step in developing a theoretical description. This technical note gives a summary of part of what has been reported in the literature.

There were four sources for acquisition of pertinent literature.

1. The report "Systems Study of Nitrogen Oxide Control Methods for Stationary Sources".

2. NAPCA publication AP-12, *Nitrogen Oxides: An Annotated Bibliography* and a computer compilation of abstracts from the Air Pollution Technical Information Center (APTIC).

3. *Chemical Abstracts* from January 1947 to October 1970.

4. Radian technical files.

Around 120 abstracts and/or articles including four doctoral dissertations were collected on the rate and mechanism of absorption. After preliminary evaluation, 50 of these

references were selected as the most valuable for a theoretical description. The 70 remaining references contained practical information such as equipment descriptions and operating conditions or empirical relationships between operating variables and absorption coefficients. Many of these references were in Russian.

Some of the 50 references of most interest were evaluated solely on the basis of the abstract. In some cases, the original articles were in Russian, Japanese, or Hungarian. A translation could not be obtained in time to include the information in this note. In other instances, the article was not available at the University of Texas Library, through the Inter-Library Loan System, or from independent libraries which usually supply photocopies. In such instances, the bibliographical reference includes the volume and number of the abstract from which information was taken.

2.0 SUMMARY OF EXPERIMENTAL STUDIES ON THE ABSORPTION RATE AND MECHANISM

The industrial production of nitric acid involves the absorption of nitrogen dioxide into water or nitric acid. Efforts to design absorption processes of high efficiency have prompted some research on factors controlling the rate of absorption. Some research on nitrogen oxides sorption has also been carried out with gas cleaning processes in mind. The published results generally involve an assumption that a certain step or process is rate controlling. Derivation of the resulting rate equations, construction of absorption equipment, collection of rate data, and demonstration that the data fit the proposed rate equation are usually described in the results. The fact remains that an adequate theoretical description of the process has not yet been given. It is not known under what conditions gas or liquid film diffusion or chemical reaction limits the rate of aqueous absorption. Further, the mechanism and kinetics of the reaction between water and nitrogen oxides have not been established.

Table I is a summary of experimental studies on the rate of aqueous NO_x absorption. Since experimental studies have been carried out under a widely varying range of conditions, an attempt has been made to present information in as uniform a manner as possible. Table I was compiled in an effort to simplify and summarize the extensive amount of data and to facilitate comparison of results obtained under different conditions.

TABLE I
EXPERIMENTAL STUDIES ON THE AQUEOUS ABSORPTION OF NITROGEN OXIDES

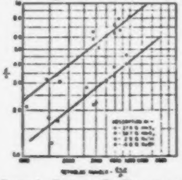
GAS COMPOSITION	ABSORBING MEDIUM	APPARATUS AND OPERATING CONDITIONS	QUANTITIES MEASURED	RESULTS AND DISCUSSION	REFERENCE
1. NO$_2$ and NO in nitrogen. Initial concentration: (gmoles/ℓ) NO$_2$ 4-12x10^{-3} NO 3-8x10^{-3} NO$_2$ = .1-.3mole% NO = .07-.2mole%	10-60% Aqueous Nitric Acid	Falling film tower, 5" long, 1.25" i.d. Gas flow rate 10-13ℓ/min. Acid rate ~ 300cc/min. Turbulent conditions liquid agitated efficiently. Maximum Reynolds number = 530.	Light absorption by NO$_2$ was measured every 30 seconds using a photocell until the system came to equilibrium. HNO$_3$ and HNO$_2$ were measured after equilibrium had been reached. [HNO$_2$] was the value obtained by titration with permanganate.	The rate of NO$_2$ removal was expressed per unit area of "acid surface". The rate was greater at 25°C than at 40°C. The rate decreased with increasing acid concentration. The rate of NO evolution was less than 1/3 the rate of NO$_2$ absorption. The rate was assumed to be limited by chemical reaction since the diffusion limiting rate equation showed the rate proportional to $P_{NO_2} + P_{N_2O_4}$ and this was not applicable. The results were expressed by Rate $= K[N_2O_4] = K[NO_2]^2$ for acids more dilute than 30%. With 30-60% acids, Rate $= K[N_2O_4] - C[N_2O_4]^{\frac{1}{2}}[NO]^{\frac{1}{3}}$.	DE-006
2. NO$_2$ - NO mixtures in N$_2$. Varying concentrations. Initial concentration: (gmoles/cm^3) NO = 1x10^{-6} N$_2$O$_4$ = 0.1-0.4 x10^{-6} NO = .025mole% N$_2$O$_4$ = .003-.012 mole%	1. H$_2$O 2. NaOH 10% 3. CaCl$_2$ soln. with vapor pressure = 75% of that over pure water.	Wetted wall column, 2.3 cm = i.d., height = 18.1 cm. Interfacial area = 128.2 ±1 cm^2. Gas Reynold's No. = 100-600.	NO$_2$ concentration was determined photometrically. N$_2$ was added from a constant pressure burette to replace the volume of gas absorbed. Photocell and gas burette readings were taken at 15-second intervals. Calculated $C_{Total} = C_T = P_{NO_2} + 2P_{N_2O_4} + P_{N_2O_3}$. Expressed rate of NO$_2$ removal as $R_{NO_2} = \left(\frac{-\Delta C_T}{\Delta t}\right)\left(\frac{\text{gas volume}}{\text{interfacial area}}\right)$	Rate of absorption into H$_2$O or dilute acid proportional to $P^2_{NO_2}$ or $P_{N_2O_4}$ if P_{NO} was low. Rate $= b[N_2O_4]$. The rate constant b was dependent on temperature and gas and liquid flow rates. If P_{NO} was higher, Rate $= b[N_2O_4]+C[N_2O_3]^n$. For absorption into alkaline solutions, Rate $= b[N_2O_4]$ when P_{NO} was low. When P_{NO} was higher, the rate of removal was much higher with alkali than with water at the same flow conditions and temperature. The rate was then described by Rate $= b[N_2O_4]+ d[N_2O_3]$. For absorption into calcium chloride, the absorption rate was lower than that into pure water. The volume of the gas space had no effect on absorption rate.	CA-014
3. NO$_2$ - N$_2$ Mixtures. Concentration NO$_2$ = 3.5-4.5 mole%.	1. 2.7-34.1% NaOH 2. 5.7-69.8% HNO$_3$	1. Wetted wall column i.d. = 1.46 cm. Reynolds No. = 1000-4900. 2. Batch absorption vessel, stirred gas passed through stirred liquid. Liquid surface 71.5 cm^2, T=25°C. Gas rate = 66 ℓ/hr.	The paper stated, "The NO$_2$ disappearing from the gas stream was calculated from the gas flow and gas analyses. Liquor analyses showed the amount of NO$_2$ absorbed when NaOH was the absorbent". It was assumed that since the liquid volume was large relative to the surface, the change in liquid concentration was small during a run. One inlet and one outlet determination were made for the gases.	The absorption coefficient d/x with d the tube diameter and x the effective film thickness was plotted vs. the Reynold's number for some of the runs as shown in Figure 5 (CH-027).  FIGURE 5. EFFECT OF GAS VELOCITY ON ABSORPTION OF NO$_2$ IN WETTED-WALL TOWER cont.	CH-027

TABLE I (cont.)

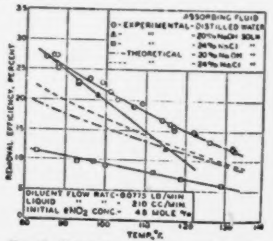
GAS COMPOSITION	ABSORBING MEDIUM	APPARATUS AND OPERATING APPARATUS	QUANTITIES MEASURED	RESULTS AND DISCUSSION	REFERENCE
3. (continued)				From this plot it was concluded that the absorption coefficient was proportional to the Reynold's number to the 0.8 power. The variation of absorption rate with concentration of NO$_2$, N$_2$O$_4$, or the absorbing medium was not discussed, although data were available to describe these variations. The ratio of film thicknesses for evaporation was plotted vs. % acid or base in absorbing medium. A maximum at pure water as the absorbing medium was interpreted to mean that the rate was greater than in acid or alkali. NO was found in the exit gas.	CH-027
4. 0.45-11.6 Vol.% eNO$_2$ eNO$_2$ = NO$_2$+ 2N$_2$O$_4$	Water and 15 wt. % HNO$_3$	Bubble-cap-plate column containing one plate. Liquid flow rates 300 and 600 cc/min., gas slot velocities = 1.18 and 2.36 ft./sec. The equipment was run until steady state flow was reached.	Liquid from the column was collected for 10-20 minutes at constant flow rates. Exit gas samples were contaminated with a mist and could not be analyzed. Liquid samples were analyzed for HNO$_3$ by titrating with standard NaOH.	The rate was assumed to be controlled by chemical reaction. The reaction $N_2O_4 + H_2O \rightleftarrows HNO_2 + HNO_3$ was assumed to describe the mechanism. The overall reaction was taken as $3/2\ N_2O_4 + H_2O \rightleftarrows 2HNO_3 + NO$ and was assumed to be irreversible under the conditions of the experiment. The resulting rate equation was $-dC_{N_2O_4}/dt = AC_{N_2O_4}$ The rate equation was integrated and the data were plotted in the form of the resulting equation with good agreement for the predicted slope.	PE-006
5. Mixture of N$_2$ and NO$_2$ containing 4.8 mole% NO$_2$.	3 solutions: distilled water NaOH-20%(wt.) NaCl-24%(wt.)	Wetted wall column 100 cm long, i.d. = 2.15 cm. Liquid flow = 210 ml/min. Temperatures from 83 to 132°F. N$_2$ flow rate = .0775 lb./min. The same liquid and gas flow rates were used for all experiments.	Liquid flow rates were determined by timed, volumetric measurements. Entering gases were sampled once and exit gases were sampled twice to determine NO. Exit liquids for distilled water and NaCl runs were titrated with standard NaOH. The removal efficiency was defined as the percent eNO$_2$ removed from the entering gas. Removal efficiency was calculated from gas and liquid flow rates and entering gas analyses and exit gas and liquid analyses.	Results are shown in the graph below. NO was found in the exit gas when NaOH was the sorbent.  Figure 2. Effect of temperature on removal efficiency	PE-007

TABLE I (cont.)

GAS COMPOSITION	ABSORBING MEDIUM	APPARATUS AND OPERATING CONDITIONS	QUANTITIES MEASURED	RESULTS AND DISCUSSION	REFERENCE
6. NO_2-N_2 mixture. 0.4-4.4 mole%. Concentration for most runs less than 1%.	Demineralized water.	30 liter glass jar, agitated liquid, gas introduced through perforated disk disperser. Bubbles released through disk were broken up by agitator. Liquid rate was 1090-1100 cc/min. Gas rate was .035-.07 lb/min. Average temperature - 25°C.	Exit liquid samples were analyzed with NaOH for HNO_3 content. Gas samples were analyzed for NO and NO_2. Results were expressed as removal efficiency of NO_2 or the percent NO_2 removed from the entering gas.	The rate equation developed previousl (PE-006) was modified to include the effects of NO. The integrated form of the rate equation predicted that a plot of results would give a series of straight lines with negative slopes and a constant intercept. The data fit the predicted form. The rate constant was predicted and found to depend on the gas-liquid contact area. Removal efficiency (%NO_2 removed from entering gas) was found to increase with gas-liquid contact area. The applicable rate equation was of the form $-dC_{eNO_2}/dt = KC_{N_2O_4} + K'C_{NO}C_{NO_2}$	PE-008
7. NO-NO_2 mixture with N_2. eNO_2 = 0.6, 1, 2, and 4 mole%. NO varied for each concentration of eNO_2 from 0 to 8.2 mole%.	Demineralized water.	Wetted wall column, 73 cm long, i.d. = 2.15 cm. Water flow rate = 270 ml/min. N_2 flow rate = .032 lb./min. Experiments carried out at room temperature.	NO and NO_2 were measured in the inlet and exit gases. Exit liquid samples were analyzed for nitrous and nitric acids. Material balances were made comparing NO and eNO_2 entering with NO, eNO_2, HNO_2 & HNO_3 leaving. N_2O_3 was found to be negligible for the material balance.	The average rate of disappearance of eNO_2 is greatur when NO is increased. When NO was high, the data did not fit the rate equation $-dC_{eNO_2}/dt = KC_{N_2O_4}$ A new mechanism was proposed involving the following reactions as the rate determining steps. $N_2O_3 + H_2O \rightleftarrows 2HNO_2$ $N_2O_4 + H_2O \rightleftarrows HNO_2 + HNO_3$ The resulting rate equation was developed. $-d(eNO_2)_g/dt = K(NO_2)_g^2 + K'(NO)_g(NO_2)_g - K''(HNO_2)_\ell^2$ The equation previously accepted (PE-006) for the overall stoichiometry was revised to include HNO_2 and was checked by using it to calculate outlet gas composition. Calculated values compared with experimental within ± 5% for most cases.	KO-024 KO-026
8. NO_2-N_2 mixtures. 5-25 mole% $\frac{NO_2 + 2N_2O_4}{\text{Total Moles}}$ = .06-.2	Deionized water.	Wetted wall column. The range of gas rates covered Reynolds numbers from 170 to 350. Water rates gave contact times from 0.03 to 0.3 sec. Temperatures were 25 and 40°C. Columns of different dimensions were used.	Exit liquid samples were analyzed by collection under NaOH and H_2O_2 and titrating with HCl. Absorbed nitrogen oxides in whatever form were reported as NO_2. The columns were operated with CO_2 and with NH_3 to establish a gas film coefficient correlation. The effects of gas rate, gas composition, contact time, and temperature on the rate were studied. Absorption rate was expressed as $\frac{\text{gmoles } NO_2}{\text{cm}^2 \text{ sec.}}$	The rate of absorption was linearly proportional to the bulk gas N_2O_4 concentration and was independent of gas velocity. The rate was also independent of contact time and slightly dependent on temperature. The data were analyzed in terms of the penetration theory and used to calculate a rate constant for the reaction between N_2O_4 and H_2O and an equilibrium constant for the physical solution of N_2O_4 in water.	WE-009

TABLE I (cont.)

GAS COMPOSITION	ABSORBING MEDIUM	APPARATUS AND OPERATING CONDITIONS	QUANTITIES MEASURED	RESULTS AND DISCUSSION	REFERENCE
9. 3-15% NO_2 in N_2	Degassed water	A wetted wall column was used with special care taken to insure laminar gas and liquid flow. Height = 13.6 cm, i.d. = 3.6 cm. Contact times of 0.2 to 0.4 seconds were used. Temperature was 25-35°C.	CO_2 and NH_3 absorptions were conducted to verify flow conditions. NO_2 was determined photometrically and HNO_2 and HNO_3 were determined from liquid samples. A mass balance was set up around the absorber. The absorption rate was expressed in gmoles equivalent NO_2/min. It was found that the difference between NO_2 entering and NO_2 leaving was 30-60% greater than the absorption rate calculated from liquid analyses. This effect was ascribed to a reaction between NO_2 and water in the gas phase.	The absorption rate was proportional to the average partial pressure of N_2O_4 in the bulk gas. The rate was considered lower than would be the case if diffusion were controlling. In developing rate expressions the gas phase reaction between N_2O_4 and water, as well as the liberation of NO were neglected. Differential equations were developed to describe NO_2-N_2O_4 diffusion and N_2O_4 dissolution and its reaction with water. The nonlinear equations were solved numerically and values for $H\sqrt{KD}$ were computed where H is the solubility of N_2O_4 in water and K is the rate of reaction of N_2O_4 and water. It was concluded that gas phase resistance would be important at higher eNO_2 concentrations but that at lower concentrations the resistance to mass transfer shifts to the liquid phase.	DE-007
10. Pure NO_2-N_2O_4 mixture (no carrier gas) Pressures from 0.06 to 0.3 atm.	Distilled, degassed water	Laminar liquid jets of 1 mm diameter and contact times of .005 and .025 seconds were formed at the tip of a thin glass tube. The water rate was 3 m/sec.	Leaving liquid was sampled and its conductivity measured to determine when steady state conditions had been reached. Liquid samples were analyzed for HNO_3 by acidimetric analysis and HNO_2 by oxidimetric analysis.	Using a previously derived equation for the rate of absorption of a dissolving gas which reacts with the solvent according to a first order reaction, the quantity $H\sqrt{KD}$ was determined for the reaction $N_2O_4 + H_2O$. Diffusion resistance in the gas phase was eliminated by using pure NO_2-N_2O_4. The rate of N_2O_4 removal was linearly proportional to its concentration at the gas-liquid interface. The decomposition of HNO_2 resulting from $N_2O_4 + H_2O \rightleftarrows HNO_2 + HNO_3$ to form NO and N_2O_4 and the subsequent reaction of N_2O_4 were taken into account. The fact that some HNO_2 was formed by the reaction of N_2O_3 and water was discussed but was not applied to the calculations.	KR-006
11. NO_2-N_2O_4 mixture in N_2	Degassed deionized water	Stirred pot - closed system surrounded by constant temperature bath. Temperatures from 0 to 70°C.	NO_2-N_2O_4 was added and the pressure change with respect to time in a closed system with constant temperature bath was measured. When pressure reached a constant value, gas samples were taken under H_2O_2 and titrated with NaOH. The absorbing solution was analyzed for HNO_3 by titrating with NaOH.	A rate equation based on the reaction $N_2O_4 + H_2O \rightleftarrows HNO_2 + HNO_3$ as the rate controlling step was developed. The measured rate was greater than the predicted one when NO was present so the rate equation was modified to the form $\text{Rate} = K(P_{NO_2})^2 + K(P_{NO})(P_{NO_2})$.	CH-028

TABLE I (cont.)

GAS COMPOSITION	ABSORBING MEDIUM	APPARATUS AND OPERATING CONDITIONS	QUANTITIES MEASURED	RESULTS AND DISCUSSION	REFERENCE
12. Not applicable	Water	Liquid N_2O_4 was injected by needle into a stream of water flowing at high velocity in a closed system. Temperatures of 2 to 20°C were used.	The temperature differentials at various points downstream from the point of injection were determined using thermocouples.	The rate of the reaction $N_2O_4 + H_2O$ was calculated and compared to values obtained from gas absorption data. (WE-009, KR-006). A mechanism for the N_2O_4 water reaction was proposed as follows with (3) the rate determining step. $O_2NNO_2 \rightleftarrows 2NO_2$ (1) $2NO_2 \rightleftarrows ONONO_2$ (2) $ONONO_2 \rightleftarrows NO^+ + NO_3^-$ (3) $NO^+ + HOH \rightleftarrows HONOH^+$ (4) $HONOH^+ \rightleftarrows H^+ + HONO$ (5) The resulting rate equation was $\frac{d[N_2O_4]}{dt} = -K_1K_2f_3[N_2O_4]$ K_1 and K_2 are the equilibrium constants for (1) and (2) and f_3 is the forward rate of step (3). $K = K_1K_2f_3$ was measured. No check was made on the validity of the rate equation.	MO-008
13. NO_2 in dilute mixtures. Concentration from 0.1 to 12%	Water	Apparatus not described. Gas velocity up to 0.5 ℓ/min. Temperature 17 to 20°C.	The optical density of a solution formed by NO_2 absorbed by 6% methanol containing 3g benzidine/ℓ was measured and found proportional to the concentration of NO_2.	An empirical relationship was developed relating log$[NO_2]$ and log α(α=degree of absorption of NO_2). There was a minimum in the plot log $[NO_2]$ *vs*. log α at 2.5×10^{-4}% NO_2.	BO-006
14. Mixtures of NO and NO_2. Concentration not described except $[NO]/[NO_2] > 1$	Solutions of NaOH, Na_2CO_3, and $NaHCO_3$	Not described in the abstract.	Not described in the abstract.	The rate of NO_2 absorption changes with the equilibrium concentration of N_2O_4 in the gas. The rate for N_2O_3 depends on its equilibrium concentration in the gas. When $[NO]/[NO_2] > 1$, the absorption is accelerated.	EL-004
15. 1. N_2O_4-NO_2 mixtures. 2. NOCl	1. $NaNO_2$ solutions. 2. Water, distilled and deareated	Laminar jet apparatus at atmospheric pressure.	In the experiments with NOCl, the concentrations of H^+, Cl^- and NO_3^- were determined by analysis of the outlet liquid. $[HNO_2]$, $[H^+]$, $[NO_3^-]$ and $[Cl^-]$ were studied as a function of NOCl pressure.	The hydrolysis mechanism was considered $N_2O_4 \rightleftarrows NO^+ + NO_3^-$ (1) $NO^+ + H_2O \rightleftarrows H^+ + HNO_2$ (2) The rate determining step was found to be (1) rather than (2). The reasons are not clearly described in the abstract. The article is unavailable at present.	MA-032

TABLE I (cont.)

GAS COMPOSITION	ABSORBING MEDIUM	APPARATUS AND OPERATING CONDITIONS	QUANTITIES MEASURED	RESULTS AND DISCUSSION	REFERENCE
16. NO-NO_2 mixtures of unspecified concentration	Na_2CO_3, $Ca(OH)_2$, and $CaCO_3$ solutions.	Apparatus not described in the abstract.	Experiments not described in the abstract.	The rates of absorption were found to increase for sorbing solutions in the order $CaCO_3$, Na_2CO_3, $Ca(OH)_2$. When Na_2CO_3 solutions were used N_2O_3 was absorbed faster than NO_2. The sorbing solution must contain at least 4 g Na_2CO_3/ℓ. The absorption rate was lowered when the density of the sorbing solution was increased by large amounts of NO_3^- and NO_2^-.	FE-010
17. Mixtures of NO_2, N_2O_4 and N_2O_3 in nitrogen. NO_2 concentration was 0.4 to 13 volume %.	Water and HNO_3	Cocurrent falling film tower 17-50°C. Gas Reynolds numbers were 600-4000. Liquid loading was 0.3-1.0 ℓ/min.	The experimental procedure was not described in the abstract.	The rate of absorption was found to be independent of the liquid velocity. The resistance was caused by the liquid phase chemical reactions. The driving force was determined by $[N_2O_4]$ and was independent of $[HNO_3]$ in the absorbing medium, the degree of oxidation of the gas phase, and the counter-diffusion of NO.	MO-004
18. Industrial gases containing NO, NO_2, and N_2O_3 in concentrations of 0.25% and higher.	Alkaline solutions	Packed columns. Gases moving at high linear velocities.	The experiments were not described in the abstract.	The rate of absorption of N_2O_3 was directly proportional to its concentration in the gas. When the gas contained equimolar quantities of NO and NO_2, the rate was proportional to their combined concentrations up to 0.25%. If both NO_2 and N_2O_3 are present, the relative proportion of NO increases. The absorption rate was found to vary as the Reynolds number to the .36 power. The absorption rate decreased as the temperature increased.	ZH-001
19. NO-NO_2 mixtures	NaOH solutions	Apparatus not described in the abstract.	Experimental conditions were not described in the abstract.	The completeness of the absorption reaction reaches a maximum at a 1:1 mole ratio of NO to NO_2. At this ratio the NO + NO_2 concentration has no effect on the completeness of reaction.	MI-005
20. NO_2-NO mixtures	Water and HNO_3 solutions	Apparatus not described in the abstract. Gas velocity was 0.3 to 5.0 m/sec. Temperatures of 20 and 50°C were used.	Experimental procedure not described in the abstract.	The rate of absorption decreased with rising temperature. At low concentrations the rate is independent of gas velocity but at some concentration it begins to depend on the velocity. When $[NO_2] > [NO]$, mostly NO_2 is dissolved. When $[NO] > [NO_2]$, mostly N_2O_3 goes into solution. The rate of absorption of N_2O_3 is 1.4 times as fast as the rate of NO_2.	ZH-002

TABLE I (cont.)

GAS COMPOSITION	ABSORBING MEDIUM	APPARATUS AND OPERATING CONDITIONS	QUANTITIES MEASURED	RESULTS AND DISCUSSION	REFERENCE
21. Equimolar mixture of NO and NO_2	Na_2CO_3, $NaNO_2$ and $NaNO_3$ solution. Total concentration of all 3 = 34-6%.	The apparatus was not described in the abstract.	The procedure was not described in the abstract.	The rate was proportional to $[N_2O_3]^{0.8}$. The absorption efficiency is sharply reduced when $[Na_2CO_3] < 3\%$. Nitrite causes a greater reduction in efficiency than nitrate. The author suggests it is due to the effect on the decomposition of HNO_2.	KR-007
22. NO mixtures in nitrogen	Solutions of Na_2SO_3, $FeCl_2$, $FeSO_4$ and $(NH_4)_2SO_3$	Static gas phase, mildly agitated liquid phase.	The experimental procedure was not described in the abstract.	Sulfite Absorption: For [NO] < .1 bar, the absorption rate was = $K_1P_{NO(g)}$ kg/m² hr. K_1 was the mass transfer coefficient. For [NO] > .1 bar, Rate = $K_1(P-P_i)_{NO}$ with P_i the equilibrium pressure at the interface. Absorption with Fe⁺⁺ Salts: The driving force expression must take into account the equilibrium: $K = [FeNO^{++}]/[Fe^{++}][NO]$	PO-014
23. Undiluted NO + NO_2 and pure NO_2	Water, HNO_3 solutions, NaOH solutions, $NaNO_3$ solutions	1. Gas bubbled through liquid. 2. Surface absorption with rapid movement of gas and liquid. 3. Surface absorption with quiet state of gas and liquid.	The experimental procedure was not described in the abstract.	For the bubbling method: Pure NO_2 and NO + NO_2 were absorbed at about the same rate. For the mixture, when NO > NO_2, the absorbate is in the form of N_2O_3. For the method of rapid gas and liquid movement: NO + NO_2 is absorbed faster than NO_2. For the method of quiet gas and liquid: N_2O_4 (pure NO_2) was absorbed much more rapidly than N_2O_3 at 25°C. The rate of absorption of N_2O_4 decreased with increasing concentration of NaOH or HNO_3. The rate for N_2O_3 decreased with increasing concentration of HNO_3. The rate for N_2O_3 increases with increasing NaOH concentration over 125g/ℓ.	AT-002
24. 80% NO_2 mixtures: 1. in N_2 2. in air 3. in N_2, O_2 with 27% NO	Water and HNO_3 solutions	A 45 mm diameter column filled with glass rings was used. Gas velocities of 0.2 mm/sec and liquid rates of 7.2 m³/m² were used.	The experimental procedure was not described in the abstract.	For mixture 1, the rate of absorption was = $K_1P_{NO_2}$ and 80-90% of the absorbed oxides formed HNO_3. For mixture 2, the rate at $P_{NO_2} > 0.5$ atm was = $KP^2_{NO_2}$. For mixture 3, only 60-75% of the oxides absorbed formed HNO_3.	TS-001
25. NO-NO_2 mixtures. Concentration not given in the abstract.	$Ca(OH)_2$ solutions.	The apparatus was not described in the abstract.	The experimental procedure was not described in the abstract.	An increase in the concentration of N oxides gave an increase in the absorption rate. The rate decreased at increasing temperatures. An increase in the volume rate of the gas decreased the absorption rate. Increasing concentration of nitrite and nitrate in solution decreased the absorption rate.	GA-008

TABLE I (cont.)

GAS COMPOSITION	ABSORBING MEDIUM	APPARATUS AND OPERATING CONDITIONS	QUANTITIES MEASURED	RESULTS AND DISCUSSION	REFERENCE
26. N oxides. No further description given in abstract	Na_2CO_3 solutions containing $NaNO_2$ and $NaNO_3$.	Packed towers - 18 m high, diameter = 7 m, temperature - 25-35°C, pressure 1.30-5 atm, gas flow rate .2-.3 m/sec, liquid flow rate 9.5 m³/m² hr. Packing was ceramic rings.	The experimental procedure was not described in the abstract.	The concentration of Na_2CO_3 had no effect on the degree of absorption at values higher than 30-35 g/ℓ. The degree of absorption decreased with increasing $NaNO_2$ and $NaNO_3$ concentration.	KR-008
27. NO, NO_2 mixture. Total concentration from 0.05 to 1.4%.	Na_2CO_3 solutions containing $NaNO_2$ and $NaNO_3$.	The apparatus is called the Penn apparatus. It is not described further in the abstract. Gas flow rates of .5-3. m/sec were used.	The coefficient of absorption efficiency is defined as equivalent N oxides absorbed/ equivalent Na_2CO_3 used. An absorption coefficient is also discussed but not defined in the abstract.	The products from sorption with Na_2CO_3 were $NaNO_3$ and $NaNO_2$. It was found that the coefficient of efficiency a) increases with increasing liquid flow rate and increasing initial concentration of N oxides, and b) decreases with increasing gas flow rate and increasing Na_2CO_3 concentration.	PO-015
28. NO_2 and N_2O_3. No concentrations given in the abstract.	5% HNO_3 solution	A rapidly revolving mechanical absorber was used. The gas velocity corresponded to a contact time of 2.4 sec. Temperature was 20-22°C. The conditions were highly turbulent.	The experimental procedure was not described in the abstract.	It was postulated that HNO_3 formation takes place via HNO_2 formation. In testing the hypothesis, the rates of NO_2 and N_2O_3 absorption by 5% HNO_3 were found to be equal.	GA-009
29. NO + NO_2 Total concentration 0.5 to 3.5%	30-199 g/ℓ Na_2CO_3 solutions	A venturi scrubber with throat diameter = 6 mm was used.	A volumetric absorption coefficient K_{Ga} in kg/m² hr. atm was determined.	The following was found concerning K_{Ga}: 1. It was a maximum at 50% conversion of NO to NO_2. 2. It decreased with decreasing concentration of N oxides in the entering gas. 3. It decreased with an increase in Na_2CO_3 concentration.	VA-006
30. NO mixtures. Concentration not given in abstract. Some NO_2 must also have been present.	HNO_3 solutions normality = 0.1, 0.01, and 0.001. HCl present to determine influence of Cl^-, normality = 0.01 to 0.04 N. Influence of Mg^{++}, Ce^{++}, Pb^{++}, Zn^{++}, and Cd^{++} also examined.	The apparatus was not described in the abstract. Temperature was 30°C.	The concentrations of HNO_2 and HNO_3 were correlated with the conductivity of their solutions. The absorption rate was expressed as the rate of formation of HNO_2.	The absorption rate was said to be controlled by the diffusion rate of HNO_2 from the gas-liquid interface to the solution. It was found that Cl^- accelerates the absorption and Mg^{++}, Pb^{++}, Zn^{++}, and Ce^{++} have negligible effect. Cd^{++} appeared to accelerate absorption. The equilibrium concentration of HNO_2 was much greater in the system NO-H_2O-HNO_3-HCl than in the system NO-H_2O-HNO_3. The original article is in Japanese.	OI-001
31. Pure mixtures of NO and NO_2. NO_2 varied from 0 to 100%. The rest was NO. Some measurements made with pure NO_2.	Water	A laminar jet apparatus was used similar to that of Kramers (KR-006, example 10). The jet diameter was 0.87 mm and the length was varied between 2 and 6 cm. The	The exit liquid was analyzed for total acid (HNO_2 + HNO_3) by quenching with a known amount of 0.1 N NaOH and back titrating with HCl. The HNO_3 content was	An empirical equation for the dependence of the total acid concentration on $[eNO_2]$, $[eNO_2]^2$, jet length, jet diameter, and water and gas flow rates was developed using regression analysis. All results were then extrapolated to a value	HO-009

TABLE I (cont.)

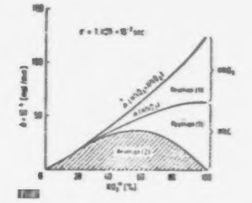
GAS COMPOSITION	ABSORBING MEDIUM	APPARATUS AND OPERATING CONDITIONS	QUANTITIES MEASURED	RESULTS AND DISCUSSION	REFERENCE
31. (cont.)		liquid flow rate was 100-130 ml/min and the gas rate was 10-40 ℓ/hr. Experiments were thermostated at 25°C.	determined separately by oxidation with $KMnO_4$ and with spectrophotometry.	of gas flow of 40 ℓ/hr and water rate of 100 ml/min. Sin[illegible] the gas contained no diluent gas, diffusion resistance was considered negligible and the rate was was considered determined by the two reactions: $N_2O_4 + H_2O \rightleftarrows HNO_2 + HNO_3$ (1) $N_2O_3 + H_2O \rightleftarrows 2HNO_2$ (2) Based on the stoichiometry of these reactions, the time rate of change of N_2O_3 and N_2O_4 were expressed in terms of the concentrations of HNO_3 and HNO_2. The results are given in the following figure.  Abb. 4 Nach Reaktion (1) und Reaktion (2) gebildete Salpetersäure und salpetrige Säure in Abhängigkeit von der Gaszusammensetzung. Verweilzeit des Strahls τ = 1,436 · 10⁻² sec It can be seen that the rate of change of N_2O_3 according to reaction 2 is greatest at 50% NO_2 and 50% NO. An equation derived previously and used by Kramers (KR-006) was used to obtain a rate constant for reaction 2. The equation is based on the penetration theory. According to the equation, the rate should be proportional to the concentration of N_2O_3 in the bulk gas. There was a deviation from linearity. The authors stated also that another possible mechanism is the gas phase formation and subsequent diffusion of HNO_2.	NO-009

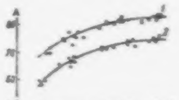
TABLE I (cont.)

GAS COMPOSITION	ABSORBING MEDIUM	APPARATUS AND OPERATING CONDITIONS	QUANTITIES MEASURED	RESULTS AND DISCUSSION	REFERENCE
32. NO-NO_2 mixtures in air. Concentration of N oxides .98-4.1%. 82% of the NO was oxidized to NO_2.	$Ca(OH)_2$ solutions concentration range 30-130g/ℓ.	A horizontal absorber containing an axial shaft to which discs were attached was used. The discs were perforated and formed blades and were rotated at high speeds to produce high gas and liquid turbulence. Countercurrent flow was used. The gas had to be separated from entrained mist after it left the absorber. Gas velocity was 400 m³ gas/m³ absorber/hr. The temperature was 30°C.	Entering and exit gases were analyzed for NO and NO_2 and the absorbing liquid was analyzed for nitrite and nitrate. The absorption coefficient Kg depended on the concentration of NO and NO_2 in the gas, the volume rate of gas flow, the speed of rotation of the discs, the temperature, and the $Ca(OH)_2$ concentration. Kg was expressed in kg/m³/hr/atm.	The rate of absorption was dependent on the concentration of nitrogen oxides at low peripheral disc speeds. At higher speeds, the absorption rates became equal for high and low initial concentrations. The rates of absorption for gases of equal concentrations containing (1) NO_2 and (2) NO_2 + NO in equimolar proportions were only slightly different in the mechanical absorber. The percent of nitrogen oxides removed from the gas stream by the mechanical absorber was reported to be higher than in commercial packed towers.	GA-010
33. Mixtures of N_2O_4 and HNO_3 in O_2.	Water	A bubble-cap column in an autoclave was used. The temperature and pressure were varied up to 90°C and 50 atm.	The measurements were not described in the abstract.	Empirical relationships be[illegible]n the rate constant for disappea[illegible] of NO_2 and temperature or pre[illegible] developed. It was found t[illegible] rate of disappearance of N[illegible] $K[NO_2]^2[H_2O]$. The propose[illegible] involved the following steps. $2NO_{2(g)} \rightleftarrows N_2O_{4(\ell)}$ (1) $N_2O_{4(\ell)} \rightleftarrows 2NO_{2(\ell)}$ (2) $2NO_{2(\ell)} + H_2O \rightleftarrows HNO_2 + HNO_3$ (3) Step 3 was proposed as rate controlling.	AT-003
34. Mixtures containing NO and NO_2. The NO was oxidized from 30 to 60% The concentration of NC + NO_2 varied up to 1.2%.	Na_2CO_3 solutions of [illegible] g/ℓ.	A column with a centrifugal sprayer was used. The liquid rate was 2.2-6.m³/m² hr and the gas rate was 167 m³/m³hr. The temperature was 10-40°C and the spray velocity was 23 m/sec.	The measurements were not described in the abstract. The degree of absorption, α, and the coefficient of absorption Kg were calculated from the data.	When 38-40% of the NO was oxidized to NO_2, the degree of absorption and the absorption coefficient increased as the concentration NO + NO_2 in the gas. With increasing temperature α and Kg decreased.	GA-011
35. Mixture of 0.5-3.5% NO + NO_2.	Na_2CO_3 solutions of 30-198.8 g/ℓ.	A turbulent gas scrubber (venturi) was used. The gas feed rate was 32-132 ℓ/min, the gas velocity was 18-78 m/sec and the liquid rate relative to the gas rate was .68-4.13 ℓ/m³.	Inlet and outlet NO and NO_2 were determined in the gas and the volumetric absorption coefficient $K_G a$ was expressed in Kg moles of N_2/m³/hr/atm. The degree of absorption was also calculated.	An empirical relationship was found for the dependence of $K_G a$ on gas velocity, liquid rate, nitrogen oxide concentration, sodium carbonate concentration and degree of oxidation of NO. The highest value of the absorption coefficient was at 50% oxidation.	VA-009

TABLE 1 (cont.)

GAS COMPOSITION	ABSORBING MEDIUM	APPARATUS AND OPERATING CONDITIONS	QUANTITIES MEASURED	RESULTS AND DISCUSSION	REFERENCE
36. Pure NO	$FeSO_4$ and $FeCl_2$ solutions, .25-.62 M in $FeSO_4$.	The apparatus was not described in the abstract. The pressure of NO was varied up to 1 atm and the temperature from 0 to 50°C.	The procedure was not described in the abstract.	Absorption is reported to take place by formation of the complex $[FeNO]^{--}_{aq}$. The results were expressed in terms of an equilibrium constant $K = \frac{V}{22.4-V} P_{NO}$ where V is the liters of NO absorbed per mole Fe^{++}. The results were independent of the concentration of $FeCl_2$.	SI-007
37. NO in nitrogen in the range 0.7-38%	$FeSO_4$ solutions from 5.6 to 20.5%.	A stirred pot reactor was used. Gas was passed over the surface of a stirred liquid at 0.2 ℓ/min. Liquid surface was 50.05 cm^2. Temperature was 20°C.	The concentration of NO in the inlet and exit gas was measured. An absorption rate and an absorption coefficient were calculated in the units kg/m^2hr and kg/m^2hr atm.	The absorption rate was linearly proportional to the concentration of NO in the gas up to 8%. At concentrations higher, the chemical capacity of the sorbent must be taken into account. The high solubility of NO in the range .7 to 8.% was proposed as the reason for the negligible liquid film resistance in that range. It was concluded that the rate of the absorption reaction process is limited by diffusion kinetics and that liquid film diffusion was negligible up to concentrations of 8-12%.	GA-012
38. Nitric oxide; 1% in nitrogen.	20% $FeSO_4$ solutions.	A packed column 510 mm high and 27.8 mm i.d. was used. The temperature was 20°C. Gas velocity was 0.09-1. m/sec.	The entering and exit concentrations of NO in the gas were measured. The absorption coefficient K_g was calculated from $Rate = K_g \Delta P$ The units of rate were kg/m^2hr and ΔP was $\log(P_{gas} - P_{liq})$, where P_{liq} was the partial pressure of NO over the liquid.	Gas film limited diffusion was assumed to be the controlling step based on the work in example 37. Therefore the influence of gas velocity on the absorption coefficient was investigated. It was found that increase of linear gas velocity resulted in an increase in the absorption coefficient and in the absorption rate. The absorption coefficient was equal to the 0.8th power of the gas velocity.	GA-012
39. Three series of experiments were conducted in which the concentrations of $NO + NO_2$ were: 1. 0.25-0.5% 2. 0.9-1.0% 3. 2.0-2.5% 65% of the N oxides were oxidized to NO_2	The absorbing medium was a solution of calcium oxide of 3-5 and 30-35 g/ℓ. The original nitrite nitrate content was varied from 50-450 g/ℓ.	A mechanical absorber similar to that described in example 32 was used. The gas rate was 400 m^3 gas/m^3hr. The peripheral disc speed was 23 m/sec and the temperature was 65-75°C.	The inlet and outlet concentrations of NO + NO_2 in the gas were measured and the percent of NO + NO_2 removed was calculated.	An increase in the calcium nitrite + nitrate concentration in the absorbing medium was found to lead to a decrease in the percent of NO + NO_2 absorbed. The relationship was not linear.	GA-014

TABLE I (cont.)

GAS COMPOSITION	ABSORBING MEDIUM	APPARATUS AND OPERATING CONDITIONS	QUANTITIES MEASURED	RESULTS AND DISCUSSION	REFERENCE
40. Two series of experiments were conducted with a mixture of $NO+NO_2$ in nitrogen in the following concentrations: 1. 0.5-0.7% 2. 1.0-1.3% The degree of oxidation of NO to NO_2 was varied from 30 to 70%.	The absorbing medium was a solution of CaO containing 4-6 g/ℓ and 200-250 g/ℓ calcium nitrate + nitrite.	The apparatus described in example 39 was used. The gas rate was 300-320 m^3/m^3hr, the peripheral disc speed was 23 m/sec and the temperature was 30-35°C.	The inlet and outlet concentrations of $NO+NO_2$ were measured and the percent of $NO+NO_2$ removed was calculated.	The percent of the nitrogen oxides absorbed increased as the degree of oxidation increased to 50%. The rate of increase diminished after the degree of oxidation reached 50%. The results are shown below.  (A) Degree of absorption (%), (B) degree of oxidation of NO (%). Concentration of NO + NO_2 (in %): 1) 1.3; 2) 0.6.	GA-014

3.0 DISCUSSION OF RESULTS

3.1 Absorption with Gases Containing NO_2 - N_2O_4

The work in Table I, numbers 3-6, 8-13, 15, 24, 26 and 33 is based on the absorption of gases initially containing only NO_2 in a range of concentrations from 0.1 to 25%. Some work was also done (numbers 10 and 23) with gases consisting of undiluted NO_2-N_2O_4. Absorbents used were water and solutions of NaOH, HNO_3, NaCl, and $NaNO_3$. Chambers and Sherwood (CH-027, Table I, number 3) concluded the rate of absorption was diffusion controlled based on a plot of tube diameter/effective film thickness vs. Reynold's number.

It has been pointed out (CA-014 and DE-006) that the rate equation for diffusion controlling shows the rate proportional to the sum of the concentrations of NO_2 and N_2O_4. Peters and coworkers (PE-006, 7, 8, and CH-028, Table I, numbers 4, 5, 6, and 11) on the other hand used a variety of equipment types and showed the absorption rate linearly proportional to the concentration of N_2O_4 or the square of the concentration of NO_2. They also demonstrated that even when no NO is added in the inlet gas, its presence must be taken into account in the rate equation due to the decomposition of HNO_3 in acid sorbents. Wendel and Pigford (WE-009) and Dekker and coworkers (DE-007) also found the rate proportional to the concentration of N_2O_4 in the gas.

Except for the work of Chambers and Sherwood (CH-027) there is general agreement that chemical reaction between NO_2-N_2O_4 and water is rate controlling. Several mechanisms for the reaction have been proposed and the rate of the reaction has been measured. Moll (MO-008) gives a good summary and discussion

of the rate measurements (DE-007, WE-009) and reports a value obtained from his own research.

Carberry (CA-015) reviewed most of the NO_2-N_2O_4 work. The equilibrium reaction

$$3NO_2 + H_2O \rightleftarrows 2HNO_3 + NO \tag{1}$$

where

$$K = \frac{P_{NO}}{P^3_{NO_2}} \cdot \frac{a^2_{HNO_3}}{a_{H_2O}}$$

had been considered a valid description of the NO_2-N_2O_4 absorption process. Data were usually plotted in the form

$$\log_{10} \frac{P_{NO}}{P^3_{NO_2}} \quad \underline{vs}. \quad \%(\text{wt.})\ HNO_3$$

Carberry plotted the data in the form $\log_{10} P_{NO}/P^{1.5}_{N_2O_4}$ and found the rate constant to be independent of temperature.

3.2 Absorption with Gases Containing NO

Table I numbers 22, 36, 37, and 38 are concerned with the absorption of pure nitric oxide or nitric oxide diluted with inert carrier gas. Absorbents used were Na_2SO_3, $(NH_4)_2SO_3$, $FeCl_2$, and $FeSO_4$. Pozin (PO-014, number 22) found that absorption rate for sulfites as the absorbent depended on the concentration of NO in bulk gas and at the gas-liquid interface. For Fe^{++} salts as the absorbent, the complex $[FeNO]^{++}$ was formed.

Sirotkin and coworkers (SI-007, number 36) also used $FeSO_4$. The abstract of the original article reported that the complex $[FeNO]^{--}_{aq}$ was formed. Since the article was a translation, it is quite possible that an error was made. Ganz (Ga-012, numbers 37 and 38) also investigated absorption using $FeSO_4$. He used a stirred pot reactor and found the absorption rate was limited by gas film diffusion.

3.2 Absorption with Gases Containing NO and NO_2

Numbers 1, 2, 7, 14, 16-21, 23-25, 27-29, 31, 32, 34, and 35 discuss absorption of gases initially containing both NO and NO_2 with the total concentration varying from .5 to 100%. Absorbents used were water and solutions of HNO_3, NaOH, $CaCl_2$, NaOH + Na_2CO_3 + $NaHCO_3$, Na_2CO_3, $NaNO_3$, Ca(OH_2), $CaCO_3$, and Na_2CO_3 + $NaNO_2$ + $NaNO_3$. There was wide agreement (PE-010, number 16; KR-007, number 21; MU-004, number 17; GA-008, number 25; KR-008, number 26) that the presence of nitrate and nitrites in the absorbent reduces the rate of absorption. Perelman (PE-010) reported the rate to increase for sorbents in the order $CaCO_3$, Na_2CO_3, $Ca(OH)_2$. Atroshchenko (AT-002, number 23) and Caudle and Denbigh (CA-014, number 2) reported the rate of absorption was faster in water than in HNO_3 or $CaCl_2$ solutions, respectively. The effect of the presence or concentration of Na_2CO_3 in the sorbing solution was investigated by several workers (VA-006, number 29; PO-015, number 27; and KR-008, number 26). Krustev (KR-008) reported that the presence of Na_2CO_3 had no effect above a lower limiting concentration. Varlamov (VA-006) stated that the absorption coefficient decreased with increasing Na_2CO_3 concentration. Pozin (PO-015) defined an efficiency coefficient as

$$\frac{\text{equivalent oxides absorbed}}{\text{equivalent } Na_2CO_3 \text{ used}}$$

and stated that the coefficient decreased with increasing Na_2CO_3 concentration.

There was general agreement (VA-009, number 35; VA-006, number 29; MI-005, number 19) that the absorption rate was a maximum at a 1:1 mole ratio of NO_2 to NO or at 50% oxidation of NO. These results are well expressed graphically by Hofmeister and Kohlhaas (HO-009, number 31).

Most workers agreed that the absorption rate was proportional to the concentration of N_2O_3 or the product of NO and NO_2 concentrations (KR-007, number 21; ZH-001, number 18; EL-004, number 14; KO-026, number 26). Perelman (PE-010, number 16) and Zhavoronkov (ZH-002, number 20) and several other workers have stated that the rate of N_2O_3 absorption is greater than the rate of N_2O_4 absorption. Atroshchenko (AT-002, number 23) found that the relative rates depended on the experimental apparatus. His results are discussed in more detail in Table I, number 23. Ganz (GA-009, GA-010) found the rates to be about equal in his apparatus (see numbers 28 and 32 and the following discussion).

Koval (KO-024, KO-026, number 7) performed an extensive investigation on the effect of adding nitric oxide on the absorption of NO_2+ N_2O_4 by water. His work seems to have been performed with great care and the mechanism he proposed explained some results found by previous workers. Although he did not measure the rates predicted by the rate equations resulting from his mechanism, he made a material balance and demonstrated that the stoichiometry resulting from his mechanism agreed with the actual stoichiometry. Some of the most significant observations in Koval's work are as follows:

1. That the absorption rate is a function of the gas-liquid contact area was demonstrated by conducting experiments in a variety of equipment types with other factors held constant.

2. In absorption experiments, the concentration of components NO, NO_2, N_2O_3, N_2O_4, HNO_2, and HNO_3 must be monitored. Early investigators assumed that the concentration of HNO_2 was negligible but Koval demonstrated its importance even when nitric oxide was not added in the inlet gas.

3. Analytical techniques are important in the NO_x-H_2O system. For instance, many investigators titrated the liquid absorption products directly with NaOH. Koval showed that decomposition of HNO_2 between the time of sampling and the analysis time could result in values for total acid from 4 to 20% too low. In addition, the titration curve for titration of nitrous acid with sodium hydroxide is not sharp since HNO_2 is always decomposing and the pH changes with time.

4. When NO and NO_2 are both present in the inlet gas, the reactions suggested by Koval to be of importance are as follows.

$$N_2O_{4(\ell)} + H_2O_{(\ell)} \rightleftarrows HNO_{2(\ell)} \quad HNO_{3(\ell)} \qquad (2)$$

$$N_2O_{3(\ell)} + H_2O_{(\ell)} \rightleftarrows 2HNO_{2(\ell)} \qquad (3)$$

Reaction 3 is faster than reaction 2 but whether it is in equilibrium is not known. The equilibrium for the second reaction in the gas phase is well described but in the aqueous phase it has not been studied extensively. An explanation (KO-026) for the fact that the second reaction

is faster than the first is that both proceed by ionization mechanisms:

$$N_2O_3 \rightleftarrows NO^+ + NO_2^- \qquad (4)$$

$$N_2O_4 \rightleftarrows NO^+ + NO_3^- \qquad (5)$$

Koval speculated that the ionization of N_2O_3 is faster than that of N_2O_4 since N_2O_4 ionization to form NO^+ and NO_3^- involves isomerization from O_2NNO_2 to $ONONO_2$.

Varlamov and Drobysheva (VA-009, number 35) tried to determine the relative effects of mass transfer and chemical reaction on the absorption of NO-NO_2 mixtures in a venturi scrubber. They used equation 6

$$\frac{1}{K_G a} = \frac{1}{k_G a} + \frac{1}{\beta H k_L a} \qquad (6)$$

to calculate βH where $K_G a$ is the overall absorption coefficient, $k_G a$ is the gas phase mass transfer coefficient and $k_L a$ is the liquid-phase mass transfer coefficient. The factor β is the coefficient representing the effect of chemical reaction and H is the Henry's Law coefficient. The mass transfer coefficients for NO + NO_2 were calculated by determining the coefficients for CO_2 in water (sparingly soluble gas, liquid phase resistance rate limiting) and SO_2 in water (highly soluble gas, resistance of gas and liquid phases comparable) and correcting for the differences in diffusion rates, viscosities, and densities of CO_2, SO_2, and NO + NO_2. It was concluded that "the boundary of chemical interaction between reacting components moves toward the liquid surface" with increasing liquid flow rate, and that "the rate is influenced by both diffusion of the active component in the gas and diffusion of the active component and the reaction product in the liquid".

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Ganz and coworkers (GA-013, GA-014) investigated the absorption of mixtures of NO and NO_2 by solutions of CaO containing calcium nitrate and calcium nitrite. The equipment used was a horizontal mechanical absorber containing a revolving axial shaft to which were connected blades or discs causing highly turbulent flow conditions. Most of the work of Ganz is generally concerned with developing empirical relationships between the absorption coefficient and hydrodynamic or physical factors with little regard for theory and mechanism. However, in the case of the mechanical absorber, discussion of a possible reaction pathway was presented. The influence of the NO_2:NO ratio in the gas and the concentration of nitrate, nitrite and CaO in the absorbing medium were investigated (see Table I, numbers 39 and 40). Some of the qualitative results are summarized in points 1 through 4.

1. Depending on the concentrations of calcium oxide, calcium nitrite and calcium nitrate, formation and precipitation of the basic salt $Ca(OH_2)_2 \cdot Ca(NO_3)_2 \cdot 2H_2O$ occurs. Gorfunkel (GO-007) also reports the possibility of formation of $CaO \cdot Ca(NO_3)_2 \cdot 2H_2O$.

2. When the nitrite-nitrate concentration in the absorbing liquor is small the presence or concentration of calcium oxide has no effect on the percent of nitrogen oxides absorbed. When the concentration of nitrite + nitrate is higher, an increase in its concentration causes a decrease in the percent of NO + NO_2 removed from the gas. An increase in the CaO concentration then retards the decrease in absorption. Ganz explained this effect by stating that in the mechanical absorber, calcium oxide is dissolved faster than $Ca(OH)_2$ can react to form nitrites and nitrates so there is an excess of

CaO rather than an excess of $Ca(NO_2)_2$. When there is an excess of the nitrite, reaction 7 takes place and NO is given off or oxidized to NO_2 thus limiting the percent absorption.

$$Ca(NO_2)_2 + 2NO_2 \rightleftarrows Ca(NO_3)_2 + 2NO \qquad (7)$$

It is proposed that in the presence of excess CaO, reaction 7 is restricted and the decrease in percent absorption is retarded.

3. It was proposed that in the mechanical absorber, reaction takes place simultaneously via NO_2 and N_2O_3 and that the rates of the two reactions are equal. The proposition is based on several observed facts.

   a. The content of NO in the exit gas was always greater than NO_2, even when the entering gas ratio NO_2:NO was ≥ 1.

   b. If only N_2O_3 absorption were taking place, the products would be totally nitrite. However, more nitrate than nitrite is formed.

4. It was proposed that in the mechanical absorber, nitrogen oxides are almost completely oxidized to NO_2 and the rate of NO_2 absorption becomes equal to the rate of N_2O_3 absorption resulting in the formation of equimolar amounts of nitrite and nitrate. The nitrite undergoes inversion according to reaction 7 and NO is liberated and oxidized in the liquid.

Andrew and Hanson (AN-001) also discussed absorption for the case of both NO and NO_2 present in the inlet gas. The authors stated that the mechanism of absorption is dependent on the relative concentrations of NO and NO_2. They described four possible absorption mechanisms and developed rate equations for a laboratory sieve plate for each mechanism. The rate equations were expressed in terms of the plate efficiency η defined as

$$\frac{\text{chemical } NO_2 \text{ absorbed}}{\text{chemical } NO_2 \text{ entering}}$$

Chemical NO_2 meant $NO_2 + 2N_2O_4 + N_2O_3 + \frac{1}{2}HNO_2$. Figure 1, taken directly from Andrew and Hanson (AN-001) shows the plate efficiencies predicted from the rate equations for each mechanism. Some physical constants had to be estimated to obtain Figure 1.

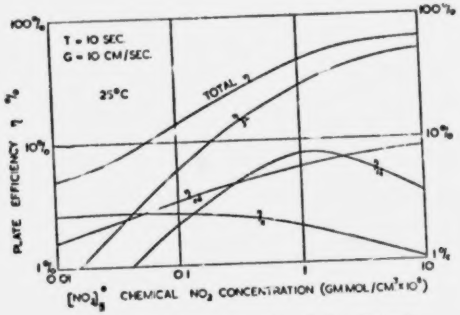

FIG. 6. Predicted component and total plate efficiencies.

FIGURE 1

In Figure 1, η_{fh}, for example, refers to the plate efficiency due to mechanism fh. The mechanisms corresponding to the alphabetic designations in Figure 1 are as follows.

Alphabetic Designation in Figure 1	Mechanism
fh	Diffusion across the gas and liquid films as NO_2 and N_2O_4. Subsequent hydrolysis of N_2O_4 to HNO_2, which decomposes to N_2O_3. $N_2O_{3(g)}$ or $HNO_{2(g)}$ given off.
e	Diffusion as NO_2, dimerization in solution, and hydrolysis of N_2O_4. $HNO_{2(g)}$ given off.
cd	Diffusion as $HNO_{2(g)}$- $N_2O_{3(g)}$ equilibrium mixture. HNO_2 decomposition in aqueous phase. NO given off.
ik	Gas phase formation of HNO_3 and HNO_2. HNO_3 both dissolves in mist and diffuses into aqueous phase. $HNO_{2(g)}$ decomposes.

Figure 2, also from Andrew and Hanson (AN-001), shows measured total plate efficiencies and shows the numerical agreement between predicted and measured values of total η. The values obtained experimentally are indicated by 0 and X, while the predicted values are indicated by the lines.

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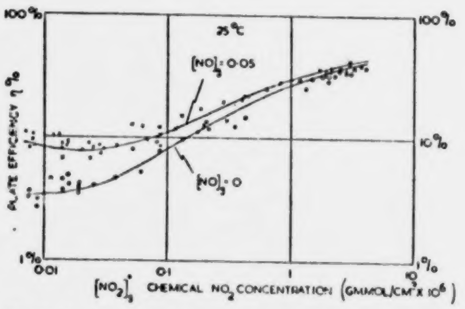

FIG. 7. A comparison of measured with predicted plate efficiencies.

FIGURE 2

From Figure 1, one can determine the controlling mechanism for this model at different gas concentrations with the relative proportions of NO and NO_2 constant. Figure 1 shows that at low gas strengths, mechanisms e and cd (diffusion as NO_2 and HNO_2-N_2O_3) are important while at higher strengths, mechanism fh (diffusion as N_2O_4 - NO_2) is most important. The point was also made that as the proportion of NO increases, mechanism cd involving N_2O_3-HNO_2 becomes more important than mechanism e involving NO_2. The contribution of mechanism ik is never important. The mechanisms operable at different gas concentrations are shown in Table II.

TABLE II

MECHANISM OF ABSORPTION AT VARYING GAS CONCENTRATIONS

GAS CONCENTRATION	MECHANISM
> .01 mole%	N_2O_4 diffusion and hydrolysis
< .01 mole%	mechanism depends on NO/NO_2 ratio
< .01 mole% ($NO/NO_2 < .5$)	liquid film limited solution of NO_2
< .01 mole% ($NO/NO_2 > 5$)	absorption and liquid phase decomposition of HNO_2
< .01 mole% ($5.0 > NO/NO_2 > 0.5$)	more than one mechanism is of importance

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TECHNICAL NOTE 200-007-03a

GAS PHASE EQUILIBRIUM IN THE SYSTEM NO_x - H_2O

23 August 1971

Prepared by:

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CHEMICAL RESEARCH • SYSTEMS ANALYSIS • COMPUTER SCIENCE • CHEMICAL ENGINEERING

This note is a modification of Technical Note 200-007-03. It includes changes made when an equation involving N_2O_5 was added to the system of equations used to describe gaseous nitrogen oxides equilibria. Note 03a is identical to Note 03 except for additions on pages 2, 3, 6, 7, 9, 10, 11, 15, 16, and 17, and corrections on pages 10 and 13.

1.0 INTRODUCTION

This note describes the chemical basis and the formulation of equations for a computer program to calculate composition in the gas phase at equilibrium. The system of interest contains nitrogen oxides, water, and their reaction products. The ability to quantitatively describe the chemical composition at equilibrium is important. With this information it is possible to predict which species are significant in the mass transfer mechanism. This note, however, describes only the chemical basis and problem formulation. The applications of the computer program and the results will be discussed in a later note.

The gas phase program was written to be compatible with the aqueous equilibrium formulation developed to describe equilibria in scrubber solutions. Ultimately, both gas and aqueous phase formulations will be used to describe equilibria in the system NO_x-CO_2-H_2O-MeO, where MeO is a metal oxide.

2.0 CHEMISTRY

In order to calculate the amount of each of the species present in the gas phase at equilibrium, the species, their possible reactions, and the resulting products must be identified. For the purposes of these calculations, the only components present in the gas phase were assumed to be the various nitrogen oxides and water, their reaction products, and inerts (see section 3). The interaction between sulfur dioxide and nitrogen oxides is a kinetics problem and was not considered.

The following species were taken into consideration

N_2O
NO
NO_2
N_2O_3
N_2O_4
N_2O_5

H_2O
HNO_2
HNO_3
O_2
N_2

The oxides N_2O and N_2O_5 are not formed in amounts great enough to be of significance for the mass balance. Even though N_2O_5 is thermodynamically unstable with respect to formation of N_2O_3 or N_2O_4 above 298°K (ST 026, p. 16), its concentration will be of significance for thermodynamic screening considerations. Both NO and NO_2 are stable with respect to decomposition into their elements.

Reaction 2-1 is slow enough to be considered the rate limiting step in nitric acid manufacture.

$$NO + \tfrac{1}{2}O_2 \rightarrow NO_2 \qquad (2\text{-}1)$$

Only 5-10% of the NO formed during combustion is oxidized to NO_2, since the residence time for most stationary combustion processes is too short (BA-003, p.1-8). Chilton (CH-032, pp.29-30) calculated 6 minutes for the time required at 43°C for reaction 2-1 to go to 95% completion at atmospheric pressure, 10% NO and 7% O_2. Therefore, the reaction was considered kinetically limited and was not included in the gas phase equilibrium formulation. Reactions 2-2 through 2-6 were included in the formulation:

$$2NO_{2(g)} \rightleftarrows N_2O_{4(g)} \qquad (2\text{-}2)$$

$$NO_{(g)} + NO_{2(g)} \rightleftarrows N_2O_{3(g)} \qquad (2\text{-}3)$$

$$N_2O_{4(g)} + H_2O_{(g)} \rightleftarrows HNO_{2(g)} + HNO_{3(g)} \qquad (2\text{-}4)$$

$$N_2O_{3(g)} + H_2O_{(g)} \rightleftarrows 2HNO_{2(g)} \qquad (2\text{-}5)$$

$$NO_{(g)} + N_2O_{5(g)} \rightleftarrows NO_{2(g)} + N_2O_{4(g)} \qquad (2\text{-}6)$$

The equilibria in 2-2, 2-3, and 2-5 have been investigated and found to be attained quite rapidly (CH-032, p.55, WA-014, WA-015, pp.11-12). Wayne and Yost (WA-014, WA-016) measured the rate of formation of HNO_2, but expressed the rate constant and the equilibrium constant for the reaction as written in 2-7,

$$NO + NO_2 + H_2O \rightleftarrows 2HNO_2 \qquad (2\text{-}7)$$

making no distinction between reactions 2-5 and 2-6 and no assumptions about the mechanism. They reported half times as short as 0.014 seconds.

Whether or not nitric acid is formed by reaction in the gas phase such as that given in 2-4 has long been a matter of some controversy. The question has been discussed by nearly every author that has written about nitrogen oxides absorption. Carberry (CA-015) summarized some of the data published up to 1959 and Wendel and Pigford (WE-009) also gave a summary and discussion of the findings of many investigators. The pertinent facts are:

(1) Many investigators have observed mist or fog formation when gaseous nitrogen oxides are absorbed into aqueous solutions. They have interpreted the mist formation as proof of a homogeneous gas phase reaction to produce $HNO_{3(g)}$ with subsequent diffusion and dissolution in water droplets. Others reported no mist formation or were able to eliminate it by filtering the carrier gas repeatedly.

(2) Nitric oxide has been found in the exit gas when sodium hydroxide was the sorbent for gases initially containing only NO_2. The sorption products of an NO_2, N_2O_4 mixture in NaOH are nitrites and nitrates; there is no unionized aqueous HNO_2 or HNO_3 present. Therefore, any NO formed could not be a result of decomposition of aqueous HNO_2. The nitric oxide must then have resulted from decomposition of gaseous HNO_2. Since no nitric oxide was present in the inlet gas, reaction 2-5 could not be the path for HNO_2 formation and reaction 2-4 must have taken place.

(3) Several investigators have attempted to observe a homogeneous reaction between water vapor and nitrogen dioxide in the absence of a condensed phase. In many cases, it was concluded that no reaction took place. The conclusions were based on the fact that either no pressure change occurred, or no mist was visible.

Wendel and Pigford (WE-009) discussed a possible explanation for mist formation and for the presence of NO in the exit gas. According to their theory, the heat of solution of highly soluble gases causes vaporization of some water. The vapor diffuses outward into the relatively cooler gas stream and condenses forming a mist or fog. N_2O_4-NO_2 mixtures can then be absorbed in the condensed water vapor forming nitric and nitrous acids. The NO is given off when nitrous acid decomposes. These workers passed N_2O_4 gas through an absorber with the gas at 25°C and the water 40°C. A dense mist was formed, but the amount of condensation decreased markedly as the gas temperature increased from 25 to 40°C.

Goyer (GO-012) reported, however, that the absorption of NO_2 in mist droplets is negligible. As suggested to him in a private communication from S. P. S. Andrew, Goyer proposed a mechanism by which gaseous HNO_3 molecules form nuclei on which water vapor condenses. The homogeneous gas phase reaction to form HNO_3 is proposed to take place between NO_2 and H_2O rather than between N_2O_4 and H_2O as in the liquid phase. A nitrogen stream saturated with NO_2 was mixed with an air stream saturated with water vapor in a mixing chamber. NO_2 was determined photometrically in the inlet and outlet gases. Apparently no condensed phase was present in the mixing chamber other than a mist which formed on mixing. Even below 20% relative humidity of the air-water vapor stream, a mist formed, but it evaporated as the temperature was slowly increased and before it could be detected on a filter. At higher relative humidities the mist was collected on a filter and analyzed for HNO_3.

Two types of experiments were run in the mixing chamber with 88% relative humidity and 4-7% NO_2-N_2O_4. The concentration of NO_2 was continuously measured photometrically. In some experiments, the gases were heated upon mixing. In these cases, the amount of mist formed was slight and remained constant. The amount of NO_2 removed increased, which was attributed to an increase in the rate of reaction between $NO_{2(g)}$ and $H_2O_{(g)}$.

In other experiments the gases were cooled on mixing. In these experiments, mist formation was quite extensive due to the condensation of water vapor. At lower temperatures the NO_2 removal decreased due to the decrease in reaction rate between $NO_{2(g)}$ and $H_2O_{(g)}$. At temperatures below the dew point, mist formation also decreased since there were few HNO_3 nuclei due to decreased reaction rate. A heavy mist

formed when NaCl nuclei were added to the gas mixture, but NO_2 removal did not increase. It was therefore concluded that NO_2 removal occurred through a gas phase reaction mechanism rather than through absorption into mist droplets.

3.0 PROBLEM FORMULATION

3.1 Description of the Method

There are i components for which we wish to calculate the mole fraction, Y_i, present at equilibrium. The components are listed below.

i	Component
1	Inerts
2	NO
3	NO_2
4	N_2O_3
5	N_2O_4
6	H_2O
7	HNO_2
8	HNO_3
9	N_2O_5

"Inerts" is used to describe flue gas components which are not considered chemically reactive in the equilibrium formulation.

The other eight components are involved in the j reactions which are also listed.

i	Reaction
1	$2NO_2 \rightleftarrows N_2O_4$
2	$NO + NO_2 \rightleftarrows N_2O_3$
3	$N_2O_4 + H_2O \rightleftarrows HNO_3 + HNO_2$
4	$N_2O_3 + H_2O \rightleftarrows 2HNO_2$
5	$NO + N_2O_5 \rightleftarrows NO_2 + N_2O_4$

The relation between the mole fraction y_i and the number of moles, n_i, for each component is defined by 3-1 where N_T is the total number of moles including inerts.

$$\sum_{i=1}^{9} y_i = \sum_{i=1}^{9} n_i/N_T = 1 \qquad (3\text{-}1)$$

In addition, we wish to define three other variables: C_{NO_2}, chemical NO_2, C_{NO}, chemical NO, and C_{H_2O}, chemical H_2O. These input variables are defined by the mass balance equations described in section 3.3.

Finally, we can write an equation for the equilibrium constant for each of the j reactions listed above. The form of the equilibrium constant expressions is given in section 3.2.

By combining the three mass balance equations and the five equilibrium constant expressions we obtain a system of eight nonlinear equations which can be solved for the eight unknowns. The system of non-linear equations is solved using an iterative procedure originally developed for solving aqueous solution equilibria.

3.2 Equilibrium Constant Expressions

The $j^{\underline{th}}$ reaction is represented by 3-2 where α and β are the stoichiometric coefficients.

$$\sum_i \alpha_{ij} \text{ Reactants} \rightleftarrows \sum_i \beta_{ij} \text{ Products} \qquad (3\text{-}2)$$

The equilibrium constant for the $j^{\underline{th}}$ reaction is shown in 3-3.

$$K_j = \frac{\prod_i a_i^{\beta_{ij}}}{\prod_i a_i^{\alpha_{ij}}} \qquad (3\text{-}3)$$

The activity, a_i, is defined as the quotient of the fugacity, f_i, of the $i^{\underline{th}}$ component and the fugacity at standard state. For a standard state of unit fugacity at one atmosphere, the activity is given by 3-4.

$$a_i \equiv f_i/f_i^{\circ} = f_i/1 = f_i \qquad (3\text{-}4)$$

Fugacities may be calculated from partial pressures using 3-5 where y_i is the mole fraction, P is the total pressure, and ν_i is the fugacity coefficient.

$$f_i = \nu_i p_i = \nu_i y_i P \qquad (3\text{-}5)$$

Substituting 3-4 and 3-5 into 3-3, taking the log of both sides, and rearranging gives 3-6.

$$\ln K_j = \sum_i \beta_{ij} \ln\left(\nu_i y_i P\right) - \sum_i \alpha_{ij} \ln\left(\nu_i y_i P\right) \qquad (3\text{-}6a)$$

$$= \left[\sum_i\left(\beta_{ij}-\alpha_{ij}\right)\right] \ln P + \sum_i \left(\beta_{ij} - \alpha_{ij}\right) \ln y_i + \sum_i\left(\beta_{ij}-\alpha_{ij}\right) \ln \nu_i \qquad (3\text{-}6b)$$

The variables are K_j, P, ν_i and y_i. The total pressure is one of the program inputs. The fugacity coefficients are very close to one for the conditions of this problem. The equilibrium constants for each of the reactions are known as a function of temperature, so they can be calculated from the input temperature (see Section 4.0). The remaining variables are the y_i's, the mole fractions which we wish to calculate.

3.3 Mass Balance Equations

Considering the stoichiometry of the reactions of interest, we can account for the chemical NO, NO_2 and H_2O by writing the mass balance equations shown in 3-7, 3-8, and 3-9.

$$C_{NO_2} = n_{NO_2} + 2n_{N_2O_4} + n_{N_2O_3} + \tfrac{1}{2}n_{HNO_2} + {}^3\!/_2\, n_{HNO_3} + 3n_{N_2O_5}$$

$$= N_T\left(y_{NO_2} + 2y_{N_2O_4} + y_{N_2O_3} + \tfrac{1}{2}y_{HNO_2} + {}^3\!/_2\, y_{HNO_3} + 3y_{N_2O_5}\right) \qquad (3\text{-}7)$$

$$C_{NO} = n_{NO} + n_{N_2O_3} + \tfrac{1}{2}n_{HNO_2} - \tfrac{1}{2}n_{HNO_3} - n_{N_2O_5}$$

$$= N_T\left(y_{NO} + y_{N_2O_3} + \tfrac{1}{2}y_{HNO_2} - \tfrac{1}{2}y_{HNO_3} - y_{N_2O_5}\right) \qquad (3\text{-}8)$$

$$C_{H_2O} = n_{H_2O} + \tfrac{1}{2}n_{HNO_2} + \tfrac{1}{2}n_{HNO_3}$$

$$= N_T\left(y_{H_2O} + \tfrac{1}{2}y_{HNO_2} + \tfrac{1}{2}y_{HNO_3}\right) \qquad (3\text{-}9)$$

The next step in the formulation is to express the total number of moles, N_T, in terms of the mole fractions and chemical NO, NO_2 and H_2O.

$$N_T = n_1 + C_{NO_2} + C_{NO} + C_{H_2O} - \left(n_{N_2O_3} + n_{N_2O_4} + \tfrac{1}{2}n_{HNO_2} + \tfrac{1}{2}n_{HNO_3} + n_{N_2O_5}\right)$$

$$= \frac{n_1 + C_{NO_2} + C_{NO} + C_{H_2O}}{1 + \left(y_{N_2O_3} + y_{N_2O_4} + \tfrac{1}{2}y_{HNO_2} + \tfrac{1}{2}y_{HNO_3} + y_{N_2O_5}\right)} \qquad (3\text{-}10)$$

Substitution of Equation 3-10 into Equations 3-7, 3-8, and 3-9 and taking the sums of Equations 3-7 + 3-8 and of Equations 3-7 + 3-9 gives the following three mass balance equations in terms of only the inputs (n_1 and chemical NO, NO_2 and H_2O) and the y_i's.

$$\frac{C_{NO_2}}{n_1 + C_{NO} + C_{NO_2} + C_{H_2O}} = \frac{\left(y_{NO_2} + 2y_{N_2O_4} + N_2O_4 + \tfrac{1}{2}y_{HNO_2} + {}^3\!/_2\, y_{HNO_3} + 3y_{N_2O_5}\right)}{\left(1 + y_{N_2O_3} + y_{N_2O_4} + \tfrac{1}{2}y_{HNO_2} + \tfrac{1}{2}y_{HNO_3} + y_{N_2O_5}\right)} \qquad (3\text{-}11)$$

$$\frac{C_{NO}+C_{NO_2}}{n_1+C_{NO}+C_{NO_2}+C_{H_2O}} = \frac{\left(y_{NO}+y_{NO_2}+2y_{N_2O_3}+2y_{N_2O_4}+y_{HNO_2}+y_{HNO_3}+2y_{N_2O_5}\right)}{\left(1+y_{N_2O_3}+y_{N_2O_4}+\tfrac{1}{2}y_{HNO_2}+\tfrac{1}{2}y_{HNO_3}+y_{N_2O_5}\right)} \tag{3-12}$$

$$\frac{C_{NO_2}+C_{H_2O}}{n_1+C_{NO}+C_{NO_2}+C_{H_2O}} = \frac{\left(y_{NO_2}+2y_{N_2O_4}+y_{N_2O_3}+y_{HNO_2}+2y_{HNO_3}+y_{H_2O}+3y_{N_2O_5}\right)}{\left(1+y_{N_2O_3}+y_{N_2O_4}+\tfrac{1}{2}y_{HNO_2}+\tfrac{1}{2}y_{HNO_3}+y_{N_2O_5}\right)} \tag{3-13}$$

The mass balance equations are solved in the log domain as are the equilibrium expressions described in 3.2. When the three mass balance equations are combined with the five equilibrium constant expressions the number of equations (8) is equal to the number of unknowns and the y_i's can be calculated.

4.0 CALCULATION OF EQUILIBRIUM CONSTANTS

As discussed in 3.2 the dependence of the equilibrium constants K_j on temperature is known. The following is a description of how K_j may be calculated. Consider the general gas phase reaction indicated by Equation 4-1, with i reactants and products where α_{ij} and β_{ij} are the stoichiometric coefficients.

$$\sum_i \alpha_{ij} \text{ Reactants} \rightleftarrows \sum_i \beta_{ij} \text{ Products} \tag{4-1}$$

Note that when i is a reactant, $\beta_i = 0$ and when i is a product, $\alpha_i = 0$. At equilibrium and at temperature T, Equation 4-2 holds.

$$\Delta G^\circ_T = \Delta H^\circ_T - T\Delta S^\circ_T \tag{4-2a}$$

$$\Delta G^\circ_T = -RT \ln K_T \tag{4-2b}$$

$$\ln K_T = -\frac{1}{R}\left(\frac{\Delta H^\circ_T}{T} - \Delta S^\circ_T\right) \tag{4-2c}$$

Thus, the equilibrium constant for a reaction at temperature T may be calculated by evaluating the right hand side of Equation 4-2c. The enthalpy term is evaluated from Equation 4-3 and likewise, the entropy term from Equation 4-4.

$$\Delta H^\circ_{T_j} = \sum_i \left\{\beta_{ij}\left[\Delta H^\circ_{f_{298_i}} + \int_{298}^{T} Cp(T)_i dT\right] - \alpha_{ij}\left[\Delta H^\circ_{f_{298_i}} + \int_{298}^{T} Cp(T)_i dT\right]\right\}$$

$$= \sum_i \left(\beta_{ij} - \alpha_{ij}\right)\left[\Delta H^\circ_{f_{298_i}} + \int_{298}^{T} Cp(T)_i dT\right] \tag{4-3}$$

$$\Delta S^\circ_{T_j} = \sum_i \left\{\beta_{ij}\left[S^\circ_{298_i} + \int_{298}^{T} \frac{Cp(T)_i}{T} dT\right] - \alpha_{ij}\left[S^\circ_{298_i} + \int_{298}^{T} \frac{Cp(T)_i}{T} dT\right]\right\}$$

$$= \sum_i \left(\beta_{ij} - \alpha_{ij}\right)\left[S^\circ_{298_i} + \int_{298}^{T} \frac{Cp(T)_i}{T} dT\right] \tag{4-4}$$

The form of Cp(T) for both products and reactants is given in Equation 4-5.

$$Cp(T) = A + BT + CT^2 - D/T^2 \qquad (4\text{-}5)$$

Integrating the heat capacity terms, substituting the temperature limits, substituting ΔH°_T and ΔS°_T in Equation 4-2c, and collecting like terms results in an equation of the following form:

$$\ell n K_T = 1/R\left(k_1 + k_2\ \ell nT + k_3T^{-2} + k_4T^{-1} + k_5T + k_6T^2\right) \qquad (4\text{-}6)$$

The form of the constants K_1 through K_6 is given below.

$$k_1 = \left[\sum_i \left(\beta_{ij} - \alpha_{ij}\right)S^\circ_{298_i}\right] + \Delta A(-\ell n\ 298.16 - 1)$$

$$+\ \Delta B(-298.16) + (-\tfrac{1}{2})(298.16)^2\ \Delta C + (-\tfrac{1}{2})\frac{\Delta D}{(298.16)^2}$$

$$k_2 = \Delta A$$

$$k_3 = (-\tfrac{1}{2})\Delta D$$

$$k_4 = (-1)\left[\sum_i \left(\beta_{ij} - \alpha_{ij}\right)\Delta H^\circ_{f_{298_i}}\right] + 298.16\ \Delta A$$

$$+\ \frac{(298.16)^2}{2}\ \Delta B + \frac{(298.16)^3}{3}\ \Delta C + \left(\frac{1}{298.16}\right)\Delta D$$

$$k_5 = (\tfrac{1}{2})\Delta B$$

$$k_6 = (1/6)\Delta C$$

where

$$\Delta A = \sum_i \left(\beta_{ij} - \alpha_{ij}\right)A_i$$

$$\Delta B = \sum_i \left(\beta_{ij} - \alpha_{ij}\right)B_i$$

$$\Delta C = \sum_i \left(\beta_{ij} - \alpha_{ij}\right)C_i$$

$$\Delta D = \sum_i \left(\beta_{ij} - \alpha_{ij}\right)D_i$$

Standard state thermodynamic properties and high temperature heat capacity data are needed to evaluate the constants k_1 through k_6. The values in Table 4-1 were used. The resulting constants for each reaction are given in Table 4-2.

TABLE 4-1

THERMODYNAMIC PROPERTIES

COMPOUND	$\Delta H^\circ_{f\,298}$ (kcal)	S°_{298} (cal)	A (cal)	B (cal x 10^3)	C (cal x 10^6)	D (cal x 10^{-5})
$HNO_2(g)$	-18.84	59.54	13.25	3.26		2.86
$HNO_3(g)$	-32.1	63.62	10.72	8.48		0.344
$H_2O(g)$	-57.77	45.07	6.78	3.57	-0.46	
$NO(g)$	21.56	50.35	7.03	0.92		0.140
$NO_2(g)$	7.91	57.34	10.26	2.04		1.61
$N_2O_3(g)$	19.80	73.91	20.50	2.05		5.14
$N_2O_4(g)$	2.17	72.72	26.09	2.72		7.95
$N_2O_5(g)$	2.70	82.80	34.24	0.79		13.40

TABLE 4-2

CONSTANTS FOR EQUATION 4-6

REACTION	K_1	K_2	$K_3 x 10^{-5}$	$K_4 x 10^{-3}$	$K_5 x 10^4$	$K_6 x 10^8$
$2NO_2 \rightleftarrows N_2O_4$	-81.664	5.57	-2.365	16.837	- 6.80	
$NO + NO_2 \rightleftarrows N_2O_3$	-56.998	3.21	-1.695	11.760	- 4.55	
$N_2O_4 + H_2O \rightleftarrows HNO_2 + HNO_3$	66.231	-8.90	2.373	- 8.661	27.25	-7.667
$N_2O_3 + H_2O \rightleftarrows 2HNO_2$	4.728	-0.78	-0.290	- 0.284	4.50	-7.667
$NO + N_2O_5 \rightleftarrows NO_2 + N_2O_4$	31.199	-4.92	1.99	11.514	15.25	

5.0 COMPARISON OF CALCULATED RESULTS WITH VALUES REPORTED IN THE LITERATURE

The object of the program is to calculate the number of moles of NO, NO_2, H_2O, N_2O_3, N_2O_4, HNO_2, HNO_3 and N_2O_5 at equilibrium in the gas phase from the input temperature, total pressure, and number of moles of NO, NO_2, and H_2O. To check the accuracy of the computational method, we must compare our calculated values with measured ones reported in the literature. The comparison should be made with values measured at more than one temperature. If possible, data from investigations of some of the individual reactions should be used.

Table 5-1 gives some of the references consulted for the reactions of interest. Most of the references are concerned with the measurement of equilibrium constants for reactions in the gas phase. Their abstracts were collected during the literature search for the entire program. As can be seen from Table 5-1, none of the experimental procedures involved measuring the concentration of gaseous species other than NO or NO_2. This is true of several other references consulted but not mentioned in Table 5-1. When it became apparent that measured equilibrium concentrations of $HNO_{2(g)}$, $HNO_{3(g)}$, $N_2O_{3(g)}$, $N_2O_{4(g)}$, $N_2O_{5(g)}$, and $H_2O_{(g)}$ had not been reported, an additional literature search was carried out. The two questions to be answered were: 1) Do analytical methods for measuring the concentrations of $HNO_{2(g)}$, $HNO_{3(g)}$, $N_2O_{3(g)}$, $N_2O_{4(g)}$, and $N_2O_{5(g)}$ exist? and 2) Have the methods been applied to measuring equilibrium concentrations of the species of interest? Chemical Abstracts Keyword Indices from 1962 to 1970 were checked and some methods for measuring low concentrations of $HNO_{3(g)}$ were found. These methods included that of Goyer (GO-012), who collected HNO_3 mist on a filter and analyzed for nitrates. However, no applications

TABLE 5-1

Experimental Measurements on Gas Mixtures at Equilibrium

Equilibrium Gas Composition	Experimental	Measured Quantities	Calculated Quantities	References
NO_2, N_2O_4	243-273°K. A bulb containing solid or liquid N_2O_4 was immersed in a thermostat whose temperature could be set between room temperature and -50°C.	P_{NO_2}, the partial pressure of NO_2 was determined spectrophotometrically.	The total pressure P in the bulb was calculated from the vapor pressure of N_2O_4 at the temperature of interest using the equations of Giaque and Kemp (GI-006). The equilibrium constant was calculated from $K_p = (P_{NO_2})^2/(P-P_{NO_2})$. The data fit the expression $\log_{10}K_p = 9.0179-2947.4/T$	VO-007
NO_2, N_2O_4, NO, N_2O_3	Solid N_2O_4 was added to NO gas and the reactants allowed to reach equilibrium in a system of known volume and temperature. The pressure was measured at temperatures from 5 to 45°C.	The pressure (at a measured volume and temperature) of NO added was reported. The amount of N_2O_4 added in grams was reported. The total pressure at equilibrium in the system (at a measured volume and temperature) was measured.	The equilibrium constant for the reaction $N_2O_3 \rightleftarrows NO + NO_2$ was calculated using (1) mass balance equations, (2) Giaque and Kemp's (GI-006) values for the equilibrium constant $K=(P_{NO_2})^2/P_{N_2O_4}$, and (3) the equation for total pressure equal to the sum of partial pressures of NO, NO_2, N_2O_3 and N_2O_4.	BE-023

TABLE 5-1 (Continued)

Equilibrium Gas Composition	Experimental	Measured Quantities	Calculated Quantities	References
NO, NO_2, N_2O_3, N_2O_4, H_2O, HNO_2, HNO_3	NO_2 was measured into a thermostatted reaction vessel. A mixture of $NO\text{-}H_2O_{(g)}$ of known composition was added. Ten minutes was allowed for equilibrium to be reached.	NO_2 added, mole fraction of H_2O in NO added, pressure at equilibrium, and equilibrium concentration of NO_2 by spectrophotometry were measured.	The equilibrium constant for the reaction $NO + NO_2 + H_2O \rightleftarrows 2HNO_2$ was calculated from (1) the measured quantities, (2) the equilibrium constants for N_2O_3 and N_2O_4 dissociation, (3) mass balance equations and the equilibrium constant for the reaction $3NO_2 + H_2O \rightleftarrows 2HNO_3 + NO$	AS-004
NO, NO_2, N_2O_4, N_2O_3, H_2O, HNO_2, HNO_3	NO, NO_2 and H_2O were isolated and allowed to reach equilibrium at ambient temperature.	The added amounts of NO, NO_2 and H_2O were measured. The amount of NO_2 at equilibrium was measured from its absorbance at 420 mμ. $HNO_{3(g)}$ was not included in the mass balance or the calculations.	The equilibrium concentrations of HNO_2, NO, N_2O_4, N_2O_3 and H_2O were calculated. The equilibrium constant for $NO + NO_2 + H_2O \rightleftarrows 2HNO_2$ was calculated.	WA-019, WA-013

to equilibrium mixtures were found. Mellor's Comprehensive Treatise on Inorganic and Theoretical Chemistry was also consulted, including a supplement on nitrogen published in 1967 (ME-009). The supplement contains a twenty-page review on the analytical chemistry of nitrogen compounds. Nothing was reported there on the determination of gaseous HNO_2 or HNO_3. Koval, who studied the absorption of NO-NO_2 mixtures in a wetted-wall column, stated (KO-026, p. 55) that analytical techniques were not sufficiently developed to allow determination of gaseous HNO_2.

Klemenc (KL-008) critically discussed four methods of analysis of gas mixtures containing NO, NO_2, N_2O_3, N_2O_4, H_2O, HNO_2 and HNO_3 in a lengthy article. None of the methods allowed the direct measurement of HNO_2 and HNO_3.

Wayne and Yost (WA-014, WA-016) measured the rate of the reaction forming $HNO_{2(g)}$ from light absorption of NO_2 measured using an electron-multiplier photo-tube and photographing the screen of a cathode-ray oscilloscope. Calculated equilibrium concentrations of $HNO_{2(g)}$ were reported as well as input H_2O and (NO_2 + N_2O_3). However, the apparatus was a flow system and the total pressure at equilibrium was not obtainable. The input NO pressure was not reported either, so calculations or comparisons could not be made with their data.

Ashmore and Tyler (AS-004, see Table 5-2) investigated the equilibrium system and reported the equilibrium concentrations of each of the species of interest. The only one of the reported values that was a measured value was the NO_2 concentration. The other values were calculated using reported equilibrium constants and mass balance equations. It was possible to calculate C_{NO}, C_{NO_2} and C_{H_2O} from the reported equilibrium

concentrations, and these inputs were used to recalculate equilibrium concentrations with the gas phase equilibrium program. A comparison of these calculated values with the reported values is shown in Table 5-2. It is obvious that the concentrations are all of the same order of magnitude.

The data of Vosper (VO-007) and Beattie and Bell (BE-023) as discussed in Table 5-1 were also used to calculate equilibrium concentrations using the equilibrium program. Vosper's data are compared with calculated values in Table 5-3 and Beattie's in Table 5-4. Note that Beattie measured only the total pressure at equilibrium. Using his reported volumes and temperatures, the number of moles present at equilibrium was derived. That number is compared with the sum of the number of moles calculated for each component by the equilibrium program.

Waldorf and Babb (WA-019) made essentially the same investigations as Ashmore and Tyler (AS-004). Again, the only equilibrium concentration measured was NO_2, and all the other reported equilibrium concentrations were calculated from equilibrium constants and mass balance equations. Waldorf and Babb ignored the formation of HNO_3 and also apparently neglected to account for the reaction of N_2O_3 to form HNO_2. They reported (WA-013) corrected values for the equilibrium constant, but they did not report the corrected equilibrium concentrations, so no calculations or comparisons could be made with their data. The data were not reported in Waldorf's dissertation (WA-015).

In summary, an attempt was made to compare measured and calculated values of equilibrium composition in the gas phase system NO_x-H_2O. The only measured equilibrium concentrations reported in the literature were for the component NO_2. The comparison of measured and calculated NO_2 partial pressures in Tables 5-2 and 5-3 showed good agreement. Measured and calculated total number of moles also agreed satisfactorily as demonstrated in Table 5-4.

TABLE 5-2

Comparison of Ashmore and Tyler's Values with Calculated Equilibrium Concentrations

	P(atm)			
	T=80.7°C		T=19.95°C	
Compound	Reported (AS-004)	Calculated	Reported (AS-004)	Calculated
NO	.5800	.5808	.6717	.6724
NO_2	.0233	.0263	.0204	.0227
N_2O_3	.00058	.00059	.0105	.0104
N_2O_4	.00007	.00012	.0045	.0049
H_2O	.13013	.13280	.0170	.0201
HNO_2	.01401	.00740	.0180	.0116
HNO_3	.000050	.000045	.000054	.000047

TABLE 5-3

Comparison of Vosper's Measured
Values with Calculated
Concentration at 273.2°K

P_{NO_2} in atm

Measured	Calculated
.067	.073
.050	.053
.031	.032
.017	.018

TABLE 5-4

Comparison of Beattie's Values
for N_T with Calculated Values

T°C	N_T Calculated by Equilibrium Program	N_T Calculated from Measured Total Pressure (BE-023)
25.04	.0358	.0353
25.04	.0345	.0341
25.04	.0395	.0391
45.12	.0144	.0152
45.04	.0452	.0463

6.0 SUMMARY

This note discussed the chemical basis for describing the equilibria established between NO, NO_2 and H_2O in the gas phase. The method of formulating the problem mathematically and solving the resulting equations for compositions was also given. Calculated values were compared when possible with measured values reported in the literature.

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TECHNICAL NOTE 200-007-04a

COMPILATION OF THERMODYNAMIC PROPERTIES FOR COMPOUNDS OF INTEREST IN NITROGEN OXIDES AQUEOUS ABSORPTION PROCESSES

7 October 1971

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This technical note contains corrections to Technical Note 200-007-04. Corrections appear on page 14 of the text and page 18 of the Bibliography. In addition Tables V and VI of the Appendix have been replaced by tables in which estimated values of nitrate and nitrite heat capacities and the heat of formation of CuO have been corrected.

1.0 INTRODUCTION

The thermodynamic properties of metal nitrates, nitrites and oxides as well as the oxides of nitrogen are necessary for calculating equilibrium constants for nitrate or nitrite decomposition reactions. These reactions are of interest in describing the thermal decomposition of nitrates and nitrites for regeneration of metal oxide sorbents for NO$_x$.

Thermodynamic data were collected for the nitrates, nitrites, nitrides, and hydroxides of 35 metals and for several nitrogen oxides. The data were compiled in a data base using a previously written program (PA-916) which also retrieves the stored data. Properties for compounds for which no experimentally determined values have been reported were estimated.

The thermodynamic properties tabulated were: the standard heat of formation and absolute entropy at 25°C; the heat capacity from 273°K to 2000°K or the data limit, whichever is lower; and the temperature, type, and heat of phase transitions.

This technical note describes the methods of data collection, the extent to which data were available, the method of storing and retrieving the data, and the methods of estimating data that were unavailable from the literature.

2.0 DATA SOURCES

The sources of the reported data were existing compilations and the open literature.

The compilations searched included:

1. JANAF Thermochemical Tables and Addendums (ST-906, ST-917, ST-918, ST-919).
2. National Bureau of Standards, Selected Values of Chemical Thermodynamic Properties (RO-907, WA-901, WA-918).
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A survey of the open literature from 1945 through January 1970 was carried out by searching Chemical Abstracts from 1947 to January 1971. It was felt that all earlier reliable values would have been reported in the compilations. The topics searched included:

alkaline earth hydroxides, nitrates, nitrides, nitrites
alkali metal hydroxides, nitrates, nitrides, nitrites
enthalpy
entropy
heat capacity

heat of formation
hydroxides
nitrates
nitric acid
nitrides
nitrites
nitrous acid
specific heat
thermodynamics

Abstracts of all promising articles from the open literature were obtained. Approximately 30 of the original articles were collected for further study. In some cases, it was necessary to extract the data directly from the abstract when the original publication was not available. If so, care was taken to insure that the bibliographic entry includes the volume and number of the abstract.

3.0 DATA STORAGE AND RETRIEVAL

A previously written computer program was used to store, tabulate, and retrieve the thermodynamic data and references. The program is also capable of calculating and plotting equilibrium constants, enthalpies, entropies, and heat capacities of specified reactions as a function of temperature.

The data for each compound of interest as well as for sulfates, sulfites, carbonates and mixed metal oxides are tabulated and printed in the Appendix in Tables V and VI. Table V contains standard heats of formation, absolute entropies, and transition data. Table VI contains heat capacity data.

4.0 CONFLICTING VALUES

Occasionally, the compilations reported widely differing values for a property of some substance. Two values were considered to be conflicting if there was greater than one kilocalorie per mole difference for the heats of formation or greater than one calorie per mole per degree K difference for the absolute entropies. In such cases, the original articles were obtained, if possible, in an attempt to resolve the conflict. One of the values was selected to be added to the data base. The selected value was accompanied by the bibliographic entry RA-001, which references this technical note and indicates that values differing from the one selected have been reported.

The following criteria have been used in selecting the values used in the data base for the heat of formation.

1. Calorimetric measurements have generally been preferred. These methods are usually the most straightforward and the experiments are normally carried out at or near room temperature. Vapor pressure or EMF measurements are usually recorded at elevated temperatures. The accuracy of conversion to standard conditions depends on availability of heat capacity data for which the authors sometimes rely [illegible]

2. Data for which the author has described his estimation of error have been preferred.

3. Values which fit best into our estimation correlation were chosen.

Criteria used in the selection of entropy values are as follows:

1. Entropy values calculated from low temperature heat capacities have been preferred over those obtained from high temperature data.

2. Values for which an error estimation was made were favored.

The selected heats of formation are discussed in Table I and the selected entropy values in Table II. Where one reference follows another in parentheses, the second reference was cited by the first author as the basis for his data. Tables I and II are included in the Appendix.

5.0 ESTIMATED THERMODYNAMIC PROPERTIES

Table III shows what data were reported in the literature for the compounds of interest. Data were tabulated for approximately 220 compounds, including hydrates. Measured heats of formation were reported for 55% of the pure compounds; measured entropies for 25%; and measured heat capacities for 20%. It was found that the nitrites as a group lacked the most data, especially for heat capacity and entropy. Since thermodynamic properties were not reported for all the compounds of interest, some of the data were estimated. Methods for estimating heats of formation, absolute entropies, and heat capacities were previously developed and had been applied to metal sulfates, sulfites, carbonates, and mixed metal oxides under Contract PH-86-68-68 to the National Air Pollution Control Administration. A detailed discussion of the methods and results has been published (PA-916).

TABLE III

THERMODYNAMIC DATA AVAILABLE FROM THE LITERATURE

CATION	ELEMENT			ANIONS OXIDE			SULFATE			CARBONATE			NITRATE			NITRITE			NITRIDE			HYDROXIDES		
	ΔH_f°*	S°	C_p*	ΔH_f°	S°*	C_p	ΔH°	S°*	C_p*	ΔH_f°	S°*	C_p*	ΔH_f°	S°	C_p	ΔH_f°	S°	C_p	ΔH_f°	S°	C_p	ΔH_f°	S°	C_p
Ag		K		K		K	K			K			K	K	K	K	K	E						
Al		K		K		K	K			E			E	E	E	E		E	K	K	K	K		
Ba		K		K		K	K			K			K	K	K	K	E	E	K	K		K		K
Be		K		K		K	K			E			E	E	E	E	E	E	K	K	K	K	K	K
Bi		K		K		K	K			E			E	E	E	E		E				K		
Ca		K		K		K	K			K			K	K	K	K	E	E	K	K	K	K	K	K
Cd		K		K		K	K			K			K	E	E	E	E	E	K			K	K	
Ce+3		K		K		K	K						E	E	E	E		E	K					
Ce+4		K		K		K	K			E			E	E	E	E		E						
Co		K		K		K	K			K			K	E	E	E	E	E				K	K	
Co+3		K																	K			K		
Cr+3		K		K		K								E	E			E	K	K	K	K		
Cr+6		K		K		E												E						
Cs		K		K			K			E			K	E	K	E	E					K		
Cu+1		K		K		K	K			E			E	E	E	E	E	E	K					
Cu+2		K		K		K	K			K			K	E	E	E	E	E				K	K	K
Fe+2		K		K		K	K			K			E	E	E	E	E	E				K		K
Fe+3		K		K		K	K			E			E	E	E	E		E				K	K	K
Ga		K		K		K								E	E			E	K	E		K	K	K
Ge(+4)		K		K		K								E	E			E	K	K				
Hf(+4)		K		K		K								E	E			E						
K		K		K		K	K			K			K	K	K	K	E	E				K	K	K
La		K		K		K	K						E	E	E	E		E	E	K				
Li		K		K		K	K			K			K	E	K	K	E	E	K	K	K	K	K	K
Mg		K		K		K	K			K			K	K	K	E	E	E	K	K	K	K	K	K
Mn+2		K		K		K	K			K			K	E	E	E	E	E			K	K	K	
Mn+3		K		K		K	K			E			E	E	E	E		E				K		
Mn+4		K		K		K								E	E			E						
Mo+4		K		K										E										
Mo+6		K		K		K									E			E						

K - known value
E - estimated value
* - not used in estimation programs

TABLE III (cont'd.)

CATION	ELEMENT			ANIONS OXIDE			SULFATE			CARBONATE			NITRATE			NITRITE			NITRIDE			HYDROXIDES		
	ΔH_f°*	S°_{298}	C_p*	ΔH_f°	S°_{298}*	C_p	ΔH_f°	S°_{298}*	C_p*	ΔH_f°	S°*	C_p*	ΔH_f°	S°	C_p	ΔH_f°	S°	C_p	ΔH_f°	S°	C_p	ΔH_f°	S°	C_p
Na		K		K		K	K			K			K	K	K	K	E	K				K	K	K
Ni+2		K		K		K	K			K			K	E	E	E	E	E				K	K	
Ni+3		K												E								K		
Pb+2		K		K		K	K			K			K	E	E	E	E	E				K	K	
Pb+4		K		K		K								E	E									
Rb		K		K			K			K			K	E	K	K	K	E				K		
Sb+3		K		K		K	K			E			E	E	E	E		E						
Sn+2		K		K		K								E	E		E	E				K	K	
Sn+4		K		K		K	K			E			E	E	E	E		E				K		
Sr		K		K		K	K			K			K	K	K	K	E	E	K			K		K
Ta+3		K																	K	K	K			
Ta+5		K		K		K									E			E						
Ti+2		K		K		K								E	E		E	E						
Ti+3		K		K		K								E	E			E	K	K	K			
Ti+4		K		K		K								E	E			E						
V+2		K		K		K									E			E						
V+3		K		K		K									E			E		K	K			
V+4		K		K		K																		
V+5		K		K		K									E			E						
W+4		K		K		K									E			E						
W+6		K		K		K									E			E						
Zn		K		K		K	K			K			K	E	E	E	E	E	K		K	K	K	
Zr+2		K												E			E			K	K			
Zr+4		K		K		K	K			E			E	E	E	E		E				K		

5.1 ESTIMATION OF HEAT OF FORMATION

Standard heats of formation were estimated for 35 metal nitrates and nitrites. Reported values for heat of formation for the corresponding metal oxides, nitrites, nitrates and carbonate or sulfate were used to estimate the unknown nitrite and nitrate heats. A computer program retrieved the 71 known heats of formation indicated by K in Table III for sulfates, carbonates, nitrates, and nitrites which had previously been stored in the data base. The program employs a method based on that of Erdös (ER-001) to perform the estimation. This method is based on the theory that the heat of reaction may be determined by summing the energies of all bonds formed during the course of the reaction. When a metal oxide (cation) i and an acid (anion) j react to form a salt, ij, the following equation may be written for estimating the heat of reaction.

$$-\Delta H^R_{ij} = B_{ij}\,(K_i - A_j)^{n_j} \qquad (1)$$

B_{ij} is the number of ion pair bonds formed, K_i is the cation combining power, A_j is the anion combining power, and n_j is the anion exponent.

The heat of formation of a salt from a_{ij} moles of cation and b_{ij} moles of anion is shown in Equation (2).

$$\Delta H^f_{ij} = a_{ij}\Delta H^f_i + b_{ij}\Delta H^f_j + \Delta H^R_{ij} \qquad (2)$$

The values for ΔH^f_i and ΔH^f_j are known; some of the ΔH^f_{ij} and thus ΔH^R_{ij} are known; a_{ij}, b_{ij}, and B_{ij}, are determined from the stoichiometry of the reaction.

Values for K_i, A_j, and n_j are obtained by correlation of existing data for ΔH^f_{ij} with a least squares technique. The solution for K, A, and n involved solving a set of 30 simultaneous nonlinear equations. Once K_i, A_j and n_j were known, ΔH^R_{ij} could be calculated and the heats of formation were estimated for desired combinations of cations and anions. Table IV gives the estimated values and the reported values on which the correlation was based. The RMS error is 2.28 cal/two ionic bonds formed.

5.2 ESTIMATION OF ABSOLUTE ENTROPIES

Absolute entropies were estimated for nitrates and nitrites for which no reported values were found. The results were based on known values for six nitrates: $AgNO_3$, KNO_3, $NaNO_3$, $Ba(NO_3)_2$, $Ca(NO_3)_2$, and $Mg(NO_3)_2$ and one nitrite, $AgNO_2$. The known and estimated values are compiled in Table V in the Appendix.

In order to estimate the nitrate and nitrite entropies, a computer program retrieved known compound entropies from the data base. It then calculated anion entropy contributions for +1 and +2-metal nitrates and +1-metal nitrites employing a modification of Latimer's method (LA-923). This method is based on subtraction of the metal or cation contribution from the compound entropy and making a correction for ionic forces. Latimer's anion entropy values for +3 and +4-metal nitrates and +2-metal nitrites (LA-923) were adopted since no data were available with which to calculate values. The anion contributions were then added to Latimer's cation values (LA-923) to obtain the estimated compound entropies.

TABLE IV

HEAT OF FORMATION AT 25 DEG C
CALORIES/GRAM MOLE

COMPOUND	I	J	PAIRS OF IONIC BONDS	CALCULATED	HEAT OF FORMATION ACTUAL	ERROR
(AG)2(CO3)	1	1	1.0	-1.2551+02	-1.2088+02	4.6241+00
(AL)2(CO3)3	2	1	3.0	-7.0876+02		
(BA) (CO3)	3	1	1.0	-2.8778+02	-2.8716+02	6.1844-01
(BE) (CO3)	4	1	1.0	-2.4740+02		
(BI)2(CO3)3	5	1	3.0	-4.7503+02		
(CA) (CO3)	6	1	1.0	-2.8561+02	-2.8811+02	-2.5065+00
(CD) (CO3)	7	1	1.0	-1.7752+02	-1.7846+02	-9.3677-01
(CE+3)2(CO3)3	8	1	3.0	-3.0810+02		
(CE+4) (CO3)2	9	1	2.0	-4.6890+02		
(CO) (CO3)	10	1	1.0	-1.7059+02	-1.7330+02	-2.7069+00
(CS)2(CO3)	11	1	1.0	-2.7291+02		
(CU+1)2(CO3)	12	1	1.0	-1.4287+02		
(CU+2) (CO3)	13	1	1.0	-1.4521+02	-1.4210+02	3.1089+00
(FE+2) (CO3)	14	1	1.0	-1.7752+02	-1.7855+02	-1.0319+00
(FE+3)2(CO3)3	15	1	3.0	-5.0442+02		
(K)2(CO3)	16	1	1.0	-2.7327+02	-2.7187+02	1.3977+00
(LA)2(CO3)3	17	1	3.0	-7.9746+02		
(LI)2(CO3)	18	1	1.0	-2.8895+02	-2.9028+02	-1.3086+00
(MG) (CO3)	19	1	1.0	-2.6033+02	-2.6338+02	-3.0579+00
(MN+2) (CO3)	20	1	1.0	-2.1044+02	-2.1374+02	-3.3082+00
(MN+3)2(CO3)3	21	1	3.0	-5.4927+02		
(NA)2(CO3)	22	1	1.0	-2.6962+02	-2.6972+02	-9.3430-02
(NI) (CO3)	23	1	1.0	-1.6889+02	-1.6298+02	5.9172+00
(PB+2) (CO3)	24	1	1.0	-1.7230+02	-1.6723+02	5.0742+00
(RB)2(CO3)	25	1	1.0	-2.7007+02	-2.6948+02	5.8583-01
(SB+3)2(CO3)3	26	1	3.0	-4.6937+02		
(SN+4) (CO3)2	27	1	2.0	-3.3132+02		
(SR) (CO3)	28	1	1.0	-2.8739+02	-2.9038+02	-2.9873+00
(ZN) (CO3)	29	1	1.0	-1.9163+02	-1.9358+02	-2.0423+00
(ZR+4) (CO3)2	30	1	2.0	-5.0327+02		
(AG)2(SO4)	1	2	1.0	-1.7117+02	-1.7036+02	8.1503-01
(AL)2(SO4)3	2	2	3.0	-8.7038+02	-8.7038+02	-1.0634-03
(BA) (SO4)	3	2	1.0	-3.4672+02	-3.4999+02	-3.2676+00
(BE) (SO4)	4	2	1.0	-2.8565+02	-2.8565+02	-4.7684-04
(BI)2(SO4)3	5	2	3.0	-6.0810+02	-6.0810+02	-3.1204-03
(CA) (SO4)	6	2	1.0	-3.3750+02	-3.4019+02	-2.6942+00
(CD) (SO4)	7	2	1.0	-2.2233+02	-2.2120+02	1.1374+00
(CE+3)2(SO4)3	8	2	3.0	-9.5300+02	-9.5300+02	-4.7684-03
(CE+4) (SO4)2	9	2	2.0	-5.6000+02	-5.6000+02	-2.5711-03
(CO) (SO4)	10	2	1.0	-2.1405+02	-2.1190+02	2.1472+00
(CS)2(SO4)	11	2	1.0	-3.4280+02	-3.3900+02	3.8013+00
(CU+1)2(SO4)	12	2	1.0	-1.7951+02	-1.7951+02	-2.9755-04
(CU+2) (SO4)	13	2	1.0	-1.8433+02	-1.8422+02	1.1356-01
(FE+2) (SO4)	14	2	1.0	-2.2110+02	-2.2041+02	6.3984-01
(FE+3)2(SO4)3	15	2	3.0	-6.1560+02	-6.1560+02	-1.0300-03
(K)2(SO4)	16	2	1.0	-3.4069+02	-3.4234+02	-1.6536+00
(LA)2(SO4)3	17	2	3.0	-9.3980+02	-9.3980+02	-4.4708-03
(LI)2(SO4)	18	2	1.0	-3.4507+02	-3.4258+02	2.4546+00
(MG) (SO4)	19	2	1.0	-3.0531+02	-3.0550+02	-1.9257-01
(MN+2) (SO4)	20	2	1.0	-2.5624+02	-2.5395+02	2.2853+00
(MN+3)2(SO4)3	21	2	3.0	-6.6690+02	-6.6690+02	-1.3539-03
(NA)2(SO4)	22	2	1.0	-3.3173+02	-3.3064+02	1.0939+00
(NI) (SO4)	23	2	1.0	-2.1139+02	-2.1350+02	-2.1120+00
(PB+2) (SO4)	24	2	1.0	-2.1874+02	-2.1933+02	-5.9867-01
(RB)2(SO4)	25	2	1.0	-3.3856+02	-3.4050+02	-1.9353+00
(SB+3)2(SO4)3	26	2	3.0	-5.7420+02	-5.7420+02	-3.4332-04
(SN+4) (SO4)2	27	2	2.0	-3.9340+02	-3.9340+02	5.8365-04
(SR) (SO4)	28	2	1.0	-3.4436+02	-3.4497+02	-6.1175-01
(ZN) (SO4)	29	2	1.0	-2.3229+02	-2.3369+02	-1.4041+00
(ZR+4) (SO4)2	30	2	2.0	-5.9701+02	-5.9701+02	-2.3534-03
(AG) (NO3)	1	3	.5	-2.8760+01	-2.9730+01	-9.6974-01
(AL) (NO3)3	2	3	1.5	-2.3938+02		
(BA) (NO3)2	3	3	1.0	-2.3723+02	-2.3711+02	1.2053-01
(BE) (NO3)2	4	3	1.0	-1.7171+02		
(BI) (NO3)3	5	3	1.5	-1.3321+02		
(CA) (NO3)2	6	3	1.0	-2.2519+02	-2.2428+02	9.1475-01
(CD) (NO3)2	7	3	1.0	-1.0858+02	-1.0906+02	-4.3268-01
(CE+3) (NO3)3	8	3	1.5	-3.0668+02		
(CE+4) (NO3)4	9	3	2.0	-3.3266+02		
(CO) (NO3)2	10	3	1.0	-1.0017+02	-1.0050+02	-3.3110-01
(CS) (NO3)	11	3	.5	-1.2015+02	-1.2180+02	-1.6523+00
(CU+1) (NO3)	12	3	.5	-3.2641+01		
(CU+2) (NO3)2	13	3	1.0	-7.0356+01	-7.2400+01	-2.0437+00
(FE+2) (NO3)2	14	3	1.0	-1.0723+02		

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( FE+3) (  NO3)3     15   3        1.5           -1.3701+02
(    K) (  NO3)      16   3         .5           -1.1817+02     -1.1770+02      4.6805-01
(   LA) (  NO3)3     17   3        1.5           -2.9933+02
(   LI) (  NO3)      18   3         .5           -1.1714+02     -1.1520+02      1.9414+00
(   MG) (  NO3)2     19   3        1.0           -1.9157+02     -1.8897+02      2.5986+00
( MN+2) (  NO3)2     20   3        1.0           -1.4260+02
( MN+3) (  NO3)3     21   3        1.5           -1.6247+02
(   NA) (  NO3)      22   3         .5           -1.1197+02     -1.1185+02      1.2035-01
(   NI) (  NO3)2     23   3        1.0           -9.7450+01     -9.9200+01     -1.7498+00
( PB+2) (  NO3)2     24   3        1.0           -1.0519+02     -1.0800+02     -2.8097+00
(   PB) (  NO3)      25   3         .5           -1.1750+02     -1.1700+02      5.0145-01
( SB+3) (  NO3)3     26   3        1.5           -1.1662+02
( SN+4) (  NO3)4     27   3        2.0           -1.6726+02
(   SR) (  NO3)2     28   3        1.0           -2.3368+02     -2.3380+02     -1.1715-01
(   ZN) (  NO3)2     29   3        1.0           -1.1829+02     -1.1560+02      2.6946+00
( ZR+4) (  NO3)4     30   3        2.0           -3.7006+02

(   AG) (  NO2)       1   4         .5           -9.5191+00     -1.0770+01     -1.2509+00
(   AL) (  NO2)3      2   4        1.5           -1.9082+02
(   BA) (  NO2)2      3   4        1.0           -1.8662+02     -1.8360+02      3.0242+00
(   BE) (  NO2)2      4   4        1.0           -1.3965+02
(   BI) (  NO2)3      5   4        1.5           -7.8172+01
(   CA) (  NO2)2      6   4        1.0           -1.8142+02     -1.7720+02      4.2225+00
(   CD) (  NO2)2      7   4        1.0           -7.0767+01
( CE+3) (  NO2)3      8   4        1.5           -2.4573+02
( CE+4) (  NO2)4      9   4        2.0           -2.5538+02
(   CO) (  NO2)2     10   4        1.0           -6.3398+01
(   CS) (  NO2)      11   4         .5           -8.8690+01
( CU+1) (  NO2)      12   4         .5           -1.6838+01
( CU+2) (  NO2)2     13   4        1.0           -3.6701+01
( FE+2) (  NO2)2     14   4        1.0           -7.0364+01
( FE+3) (  NO2)3     15   4        1.5           -6.8566+01
(    K) (  NO2)      16   4         .5           -8.9187+01     -8.9480+01     -2.9322-01
(   LA) (  NO2)3     17   4        1.5           -2.7995+02
(   LI) (  NO2)      18   4         .5           -9.3264+01     -9.6600+01     -3.3361+00
(   MG) (  NO2)2     19   4        1.0           -1.5363+02
( MN+2) (  NO2)2     20   4        1.0           -1.0401+02
( MN+3) (  NO2)3     21   4        1.5           -1.1156+02
(   NA) (  NO2)      22   4         .5           -8.4993+01     -8.5720+01     -7.2736-01
(   NI) (  NO2)2     23   4        1.0           -6.1397+01
( PB+2) (  NO2)2     24   4        1.0           -6.6096+01
(   PB) (  NO2)      25   4         .5           -8.8881+01     -8.8710+01      1.7099-01



( SB+3) (  NO2)3     26   4        1.5           -7.0209+01
( SN+4) (  NO2)4     27   4        2.0           -1.0998+02
(   SR) (  NO2)2     28   4        1.0           -1.8568+02     -1.8220+02      3.4773+00
(   ZN) (  NO2)2     29   4        1.0           -9.3575+01
( ZR+4) (  NO2)4     30   4        2.0           -2.9116+02


           ROOT MEAN SQUARE ERROR =  2.2809+00    CALORIES/PAIR OF IONIC BONDS
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The RMS errors for the estimated +1-metal nitrate and the +2-metal nitrates were respectively 0.925 and 2.62 entropy units.

5.3 ESTIMATION OF HEAT CAPACITIES

Heat capacity coefficients for metal nitrates and nitrites whose corresponding oxide heat capacities were known have been estimated. The results were based on reported heat capacity data for the nitrates, nitrites, and oxides of seven metals as shown in Table III.

The estimation method used for the nitrates involved adding an increment, ΔC_p, to known oxide heat capacities. The increment was calculated by a computer program by subtracting oxide heat capacity coefficients from known nitrate heat capacity coefficients. Using a least squares method, an average nitrate increment was obtained. The increment ΔC_p was then added to each set of oxide coefficients yielding an estimated nitrate heat capacity. The temperature range of validity for the estimated coefficients was taken to be that of the coefficients for the corresponding oxide. The same method was applied to the estimation of nitrite heat capacities.

The accuracy of this estimation technique was indicated by the fractional error, which is defined as the RMS error divided by the average known heat capacity for the group of compounds of interest. For the nitrate correlation, the fractional error was 0.208. The fractional error for the nitrite correlation could not be estimated on the basis of one compound. The estimated values were added to the data base. Table VI is a compilation of known and estimated heat capacity coefficients. It is included in the Appendix.

6.0 SUMMARY

Thermodynamic data were compiled for 220 compounds including the pure and hydrated nitrates, nitrites, nitrides, and hydroxides of 35 metals plus several nitrogen oxides. Data were collected and evaluated from the compilations and the open literature. When widely differing values were reported, one value was selected after consulting the original references. Standard heats of formation and absolute entropies were estimated for nitrates and nitrites for which no data were reported. Coefficients for heat capacity equations were estimated for 39 nitrates and 45 nitrites for which no data were reported. The accuracy of each correlation was determined by comparing accepted values with those calculated by each method and computing a root mean square (RMS) error. The estimated values were also compiled in the data base. A copy of the data base arranged in alphabetical order is contained in the Appendix in Tables V and VI. Table V contains the standard heats of formation, absolute entropies, and transition data; Table VI is a tabulation of the heat capacity data. Tables I and II are also included in the Appendix. They contain a description of values selected for heat of formation and entropy when widely differing reported values were found.

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TR-005 HEAT OF FORMATION OBTAINED BY COMBINING HEAT OF REACTION FROM LITERATURE WITH HEATS OF FORMATION FROM TRACOR DATA BASE.

TR-006 ABSOLUTE ENTROPY OBTAINED BY COMBINING ENTROPY OF REACTION FROM LITERATURE WITH ABSOLUTE ENTROPIES FROM TRACOR DATA BASE.

TR-007 ENTROPIES FOR TUNGSTATES AND MOLYBDATES ESTIMATED FROM OBSERVATIONS BASED ON RESULTS IN TECHNICAL MEMORANDUM 004-009-CH5.

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APPENDIX

TABLE I

CONFLICTING VALUES FOR THE STANDARD HEAT OF FORMATION OF INORGANIC COMPOUNDS

COMPOUND	VALUE(KCAL/MOLE)	REFERENCE	REMARKS	ACCEPTED VALUE(KCAL/MOLE)
$Mn(NO_3)_2$	-137.73	WA-901, WA-912 (EW-901)	Both reported values were based on the same data, but they differ by approximately 30 kcal. Ewing (EW-901) calorimetrically measured the heat solution and the heats of dilution up to 24m for $Mn(NO_3)_2$. Guntz (GU-911) also measured the heat of solution. In a private communication (WA-912) Wagman stated the reference used in his compilation (WA-901), but did not cite the values used to calculate the heat of formation from Ewing's solution data. Rossini (RO-907) gave no further information concerning the calculation of his value. The value which agreed closest with the Radian estimate (RA-002) was accepted.	-137.73
	-137.73	ST-926 (WA-901)		
	-166.32	RO-907 (EW-901,GU-911)		
	-142.6	RA-002		

TABLE I (cont'd.)

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COMPOUND	VALUE(KCAL/MOLE)	REFERENCE	REMARKS	ACCEPTED VALUE(KCAL/MOLE)
$Fe(NO_3)_3 \cdot 9H_2O$	-785.2	WA-901, WA-912 (BE-928)	All three reported values were based on Berthelot's measurements. Landolt-Boernstein (LA-908) cites Rossini's; but Rossini's compilation (NBS Circular 500) was revised by Wagman (WA-901). The most recently calculated value was adopted.	-785.2
	-784.4	RO-907 (BE-928)		
	-783.7	LA-908 (RO-907)		
$CsNO_3$	-121.8	ST-926 (WA-901, WA-918)	Stern (ST-926) cites an unpublished value of Wagman's NBS compilation series (WA-901, WA-918). This series is an ongoing revision of NBS Circular 500 (RO-907) which reports a value in agreement with that given by Landolt-Boernstein. The revised value was accepted.	-121.8
	-118.1	LA-908		
	-118.11	RO-907		
$Co(NO_3)_2$	-100.5	WA-901, WA-912 (GU-911)	Plekhotkin (PL-903) stated that the value he gives has been reported in reference books, but he does not give the reference. Guntz (GU-911) measured the heat of dissolution of $Co(NO_3)_2$ by calorimetry; his data served as the basis for determinations of the heat of formation by Rossini (RO-907) and Wagman (WA-901, WA-912). Both are National Bureau of Standards	-100.5
	-102.9	RO-907 (GU-911)		
	-102.9	PL-903		

TABLE I (cont'd.)

COMPOUND	VALUE(KCAL/MOLE)	REFERENCE	REMARKS	ACCEPTED VALUE(KCAL/MOLE)
			publications, but Wagman's technical notes are an ongoing revision of Rossini's compilation. Wagman's value was adopted.	
$Ni(NO_3)_2$	-99.2 -102.2 -101.5	WA-901, WA-912 (GU-911) RO-907 (GU-911) PL-903	See remarks for $Co(NO_3)_2$.	-99.2
$Ca(NO_2)_2$	-177.2 -178.3 -178.3	ST-926 (WA-918) RO-907 (DO-910) PL-903	Stern (ST-926) cites a value reported by Wagman (WA-918) who is in the process of revising NBS Circular 500 (RO-907). However, $Ca(NO_2)_2$ was not included in Wagman's compilation. In Stern's bibliography there was a statement that sometimes	-177.2

TABLE I (cont'd.)

COMPOUND	VALUE(KCAL/MOLE)	REFERENCE	REMARKS	ACCEPTED VALUE(KCAL/MOLE)
			he reported values of Wagman not yet published. Assuming that this was the case for $Ca(NO_2)_2$ Stern's value was accepted. Plekhotkin's reference is not clear (see remarks for $Co(NO_3)_2$).	
$Ba(NO_2)_2$	-183.6 -174.0 -187.6	ST-926 (WA-918) RO-907 (BE-928, BE-930, BU-918, DO-910, DO-911) PL-903	See remarks for $Ca(NO_2)_2$. Stern's value was accepted.	-183.6
Ba_3N_2	-86.9±8 -86.9 -89.10±21 -89.900	KU-903 (RO-907) RO-907 (GU-904) LA-908 (WE-919 [GU-904]) KE-911 (LA-916 [GU-904])	Guntz (GU-904) in his 1923 article describes his determination of the heat of formation. The heat of solution of Ba_3N_2 in hydrochloric acid was measured by calorimetry. The data were then employed in a Hess cycle to obtain the heat of formation. Landolt-Boernstein (LA-916, LA-908), Kubaschewski (KU-903), Rossini (RO-907), and Kelley (KE-911) all base their values on Guntz's data, using redetermined values in the cycle.	-86.9

COMPOUND	VALUE(KCAL/MOLE)	REFERENCE	REMARKS	ACCEPTED VALUE(KCAL/MOLE)
			Kubaschewski's value was adopted here because 1) the author states an error estimate, and 2) Landolt-Boernstein references an early Kubaschewski work (WE-919) which was later revised.	
AlN	-76.0	ST-906 (NE-907, MA-946)	The JANAF Thermochemical Tables (ST-906) adopted an average of the values reported by Neubauer and Margrave (NE-907) in 1957 and by A.D. Mah (MA-946) in 1961, both of which were obtained by calorimetric measurements. Kubaschewski (KU-903) and Landolt-Boernstein (LA-908), having accepted Neubauer's data, agree closely with the JANAF value; In 1932, Neumann, Kroger, and Haebler (NE-908) reported a much lower value, which was adopted by Kelley (KE-911) and Rossini (RO-907). The latter, a National Bureau of Standards publication, has recently been revised by Wagman (WA-918), who agrees with the JANAF tables. In a 1962 article, Dreger and coworkers (DR-901) reviewed the heat of formation data published for AlN, and they stated that Neumann's data are in error, but do not give any reason for this decision. Linevsky (LI-908) recently reported a value determined by	-76.0
	-76.0	WA-918		
	-76.5±1.0	KU-903 (NE-907)		
	-76.48	LA-908 (NE-907)		
	-57.7	RO-907 (NE-908)		
	-57.4	KE-911 (NE-908)		
	-71.8±2	LI-908		

COMPOUND	VALUE(KCAL/MOLE)	REFERENCE	REMARKS	ACCEPTED VALUE(KCAL/MOLE)
			vapor pressure measurements; only the abstract of this article was obtained The JANAF value was adopted.	
TiN	-80.7±1	ST-919 (HU-908, NE-909)	The most recent JANAF value (ST-919) was selected because Stull averages Humphrey's latest data (HU-908), Humphrey's data corrected for anatase, and Neumann's data (NE-909). This includes nearly all the reported values. The earlier JANAF value (ST-906) was revised by Stull. Hoch's data (HO-919) were rejected by Stull because of large uncertainties in comparison to Humphrey's calorimetric data (HU-903, HU-908, HU-909).	-80.7
	-80.5±1.5	ST-906 (NA-935)		
	-80.4±0.8	KU-903 (HU-908, HU-909, HU-903, WE-919)		
	-79.4	LA-908 (HO-919)		
	-73.0	RO-907 (NE-909)		
	-80.2±0.2	MA-943 (HU-908)		
VN	-51.9±2.5	KU-903 (MA-947, MA-948)	Slade and Higson (SL-905, SL-906) studied the thermal dissociation of VN. Kelley (KE-911) applied an estimated entropy value to Slade's data to obtain the heat of formation. Kelley's data are rejected because they are based on an estimated value. Mah's reports (MA-947, MA-948) did not contain any data on the compound in question. Therefore, we could not accept Kubaschewski's data.	None
	-41.42	LA-908 (KE-911)		
	-41.	RO-907 (KE-911)		
	-41.430	KE-911 (SL-905, SL-906)		

TABLE I (con'td.)

COMPOUND	VALUE(KCAL/MOLE)	REFERENCE	REMARKS	ACCEPTED VALUE(KCAL/MOLE)
Cr$_2$N	-30.5	WA-901 (MA-943)	A.D. Mah (MA-943) measured the heat of formation of Cr$_2$N by combustion calorimetry. She reviewed the data previously reported by Sano (SA-916) and Seybolt and Oriani (SE-910), stating that their results could not be compared with her own since no heat capacity data are available for the temperatures at which they worked. Sano's article has not been translated from Japanese, and so was not read. Seybolt and Oriani measured the solubility and activity of nitrogen in the Cr-N solid solution. Rossini (RO-907) adopted the data of Sano, but Wagman recently revised that compilation, and based his value on Mah's work. Landolt-Boernstein referenced a 1959 work of Kubaschewski, who later revised this value upward and reduced the error estimate. T. Mills (MI-906) carried out a thermogravimetric study of the compound in question. However, we were not able to investigate this source further because the report was not available. The accepted value was Wagman's, based on Mah's research.	-30.5
	-23.4	RO-907 (SA-916)		
	-27.3±0.8	KU-903		
	-25.30±14	LA-908 (KU-906)		
	-26.72	MI-906		
	-30.8±1.1	MA-943		
	-23.500	SE-910		

TABLE I (cont'd.)

COMPOUND	VALUE(KCAL/MOLE)	REFERENCE	REMARKS	ACCEPTED VALUE(KCAL/MOLE)
Mn$_8$N$_2$	-61.5	WA-901, WA-912 (MA-933)	Wagman (WA-901) and Landolt-Boernstein (LA-908) base their values on experimental work carried out by A. D. Mah. Her report (MA-933) was read; she determined the heat of formation of Mn$_4$N by combustion calorimetry to be -30.3±0.4 kcal, which Landolt-Boernstein apparently doubled to get ΔH°_f for Mn$_8$N$_2$. In a private communication (WA-912), Wagman states the source of his data, but does not describe calculations employed. It seems possible that, after doubling ΔH°_f for Mn$_4$N, an additional increment was added to account for a heat of reaction for $2\ Mn_4N \rightleftarrows Mn_8N_2$ Rossini's value was rejected because 1) Mah's data had not yet been published, and 2) Wagman's compilation updates the 1952 value. Wagman's value was adopted.	-61.5
	-60.6	LA-908 (MA-933)		
	-81.	RO-907 (SA-917)		
Mn$_5$N$_2$	-48.2±0.6	MA-933	A. D. Mah (MA-933) determined the heat of formation of Mn$_5$N$_2$ by bomb calorimetry. Her results were published in 1958, six years after Rossini's compilation (RO-907). Although Wagman's (WA-901) source was not reported, it appears that it probably was Mah's data. Mah's original results were accepted.	-48.2
	-48.2	LA-908 (MA-925)		
	-48.8	WA-901		
	-57.8	RO-907 (NE-908, NE-910, SA-917)		
	-57.77	KE-911 (NE-909)		

COMPOUND	VALUE(KCAL/MOLE)	REFERENCE	REMARKS	ACCEPTED VALUE(KCAL/MOLE)
Zn_3N_2	-5.4	WA-918	RO-907 was eliminated since Juza's value (JU-902), obtained by solution calorimetry was high compared to other reported values. Landolt-Boernstein (LA-908) and Kubaschewski (KU-903) adopt a value reported earlier by Weibke and Kubaschewski (WE-919) which was unavailable. Wagman's revision (WA-918) of Circular 500 (RO-907) is the accepted value because it is the most recently redetermined value.	-5.4
	-6.9	RO-907 (JU-902)		
	-5.3±2.0	KU-903(WE-919)		
	-5.31	LA-908 (WE-919)		
Mo_2N	-19.5±0.3	MA-943	The values reported in the compilations are based on two similarly conducted experiments done by Mah (MA-943) and Neumann and co-workers (NE-909). The heat of combustion of Mo_2N was measured using bomb calorimetry; $Mo_2N_{(c)}+3O_2(g) \rightarrow 2MoO_3(c)+\frac{1}{2}N_2(g)$. Mah combined this value with her previously determined standard heat of formation of MoO_3 to obtain the heat of formation for the nitride. Neumann also measured the heat of reaction for the combustion of molybdenum metal.	-19.5
	-19.50	WA-901, WA-912 (MA-943)		
	-16.6±2.1	LA-908 (KU-906 [NE-909])		
	-16.6 ±0.5	KU-903 (KU-907 [NE-909])		
	-16.6±0.6	NE-909		

COMPOUND	VALUE(KCAL/MOLE)	REFERENCE	REMARKS	ACCEPTED VALUE(KCAL/MOLE)
			$2Mo + 3O_2 \rightleftarrows 2MoO_3$ By combining the two equations, he obtained the heat of formation for Mo_2N. Mah's value was accepted because of the higher purity of the Mo_2N used and availability of the standard heat of formation of MoO_3.	
Be_3N_2	-140.6±0.3	ST-918 (GR-911)	The ΔH°_f in the JANAF Thermochemical Tables (ST-918, ST-906) is a weighted mean value of data from Gross, et al. (GR-911) and the same data with JANAF's corrected value for ammonia. Gross and coworkers measured the heat of chlorination of α-Be_3N_2 to α-$BeCl_2$, and the heat of reaction of Be with ammonia. Hoenig and Searcy (HO-910) have investigated the decomposition reaction. $Be_3N_2(c) = 3Be_{(g)} + N_2(g)$ using the Knudsen technique. Stull, using 2nd and 3rd law methods, analyzed the data obtained and rejected the results (ST-918).	-140.6
	-140.6±0.6	ST-906 (GR-911)		
	-136. ±6	HO-910		
	-134.70	LA-908 (KU-906)		
	-134.7±5.0	KU-903 (WE-919)		
	-135.7	RO-907 (NE-908, NE-909)		
	-133.5	KE-911 (NE-908)		

TABLE I (cont'd.)

COMPOUND	VALUE(KCAL/MOLE)	REFERENCE	REMARKS	ACCEPTED VALUE(KCAL/MOLE)
			Landolt-Boernstein (LA-908) adopted a value reported by Kubaschewski and Evans (KU-906) in 1959. However, in Kubaschewski's 1967 compilation, a 1943 value reported by Weibke and Kubaschewski (WE-919) was adopted and a large error estimate was given. The original literature was not obtained. Kelley's 1937 compilation (KE-911) cited an out-of-date 1936 Landolt-Boernstein publication based on data reported by Neumann, Kroeger and Haebler (NE-908). Rossini (RO-907) accepted a combination of data reported by Neumann et al. (NE-908, NE-909). The accepted value was JANAF's.	
Sr_3N_2	-91.3±4. -93.4±5.0 -93.4	LA-908 (WE-919) KU-903 (RO-907) RO-907 (GU-904)	The value reported in Kubaschewski's later compilation (KU-903) and in NBS Circular 500, (RO-907) based on solution calorimetry data of Guntz and Benoit (GU-904) was accepted. Landolt-Boernstein (LA-908) adopted	-93.4

TABLE I (cont'd.)

COMPOUND	VALUE(KCAL/MOLE)	REFERENCE	REMARKS	ACCEPTED VALUE(KCAL/MOLE)
			a value reported in 1943 by Weibke and Kubaschewski (WE-919). The latter was unavailable. Thus, no check on the original source could be made.	
TaN	-60.0±.6 -59.0±1.2 -58.2	LA-908 (MA-949) KU-903 (MA-949, KU-907, [NE-909]) RO-907 (NE-909)	Mah and Gellert (MA-949) determined the heat of formation of TaN by combustion calorimetry. Landolt-Boernstein (LA-908) accepted this value without any corrections. Kubaschewski (KU-903) however adopted a value obtained by averaging Mah's data with that reported by Neumann, Kroger and Kunz in 1934. Rossini's value (RO-907) based on Neumann's data was not accepted because at the time of publication of his work, Mah's data were not available. Kubaschewski's average was accepted.	-59.0
$Mg(OH)_2$	-221.0±0.5 -221.0±0.7 -221.0 -220.9 -8.85±0.2	ST-918 ST-906 RO-907 LA-908 KU-903 (RO-907)	Since Kubaschewski's value seemed questionable, we checked his source, NBS Circular 500 (RO-907). But the reported value did not agree with the value reported by Kubaschewski.	

COMPOUND	VALUE(KCAL/MOLE)	REFERENCE	REMARKS	ACCEPTED VALUE(KCAL/MOLE)
			After eliminating Kubaschewski's value, we selected the value agreed upon by Stull (ST-906, ST-918) and Rossini (RO-907).	
$Ca(OH)_2$	-237.5±1.5	KU-903 (HA-936)	Kubaschewski's value (KU-903) was accepted here because 1) Hatton's (HA-936) is the most recently determined value (1959) and 2) he is the only author to give limits of accuracy. Note that Hatton's data were not available to Rossini at the time of publication of his compilation (RO-907) in 1952.	-237.5
	-235.7	LA-908 (RO-907)		
	-235.8	RO-907 (TA-911, SC-919, SC-920, MO-913)		
$Fe(OH)_2$	-137.2±0.7	ST-918 (FR-913)	Fricke and Rihl (FR-913) investigated the heat of combustion for the reaction $Fe(OH)_2(c)+\frac{1}{4}O_2(g)=\frac{1}{2}Fe_2O_3(c)+H_2O_{(l)}$ and found it to be -29.8±0.65 kcal/mole. From these data Stull (ST-918) determined the heat of formation, including an estimate of error. J. Thomsen (TH-908) measured the enthalpy changes of the following reactions:	
	-136.0	WA-901, WA-912 (FR-913, TH-908)		
	-135.8	RO-907 (FR-913, TH-908)		
	-135.8	LA-908 (RO-907)		

COMPOUND	VALUE(KCAL/MOLE)	REFERENCE	REMARKS	ACCEPTED VALUE(KCAL/MOLE)
			Reaction — $\Delta H°R$, 291° $FeCl_2(c)=FeCl_2(400\ H_2O)$ — -17.9 kcal/mole $FeCl_2(200\ H_2O)+H_2SO_4(200\ H_2O)= FeSO_4(200\ H_2O)+2HCl(200\ H_2O)$ — -3.6 kcal/mole $FeSO_4(aq)+2KOH(aq)= Fe(OH)_2(c)+K_2SO_4(aq)$ — -6.34 kcal/mole Stull, in his discussion of $Fe(OH)_2$, refers to Thomsen's data. He points out that Thomsen's results depend on the assumption that in his second reaction, 200 moles of water are present. Stull rejects the data on this basis. Using the data of Fricke and Rihl and Thomsen, Rossini (RO-907) calculated $\Delta H°_f$. This value has been redetermined by Wagman (WA-901). We agree with Stull's comments, and accept the value he reports based on Fricke and Rihl's data.	

COMPOUND	VALUE(KCAL/MOLE)	REFERENCE	REMARKS	ACCEPTED VALUE(KCAL/MOLE)
Co(OH)$_2$	-129.4	GE-903	Gedansky, Bertrand, and Hepler (GE-903) recently determined the heat of formation of Co(OH)$_2$ from calorimetric measurements of the heats of precipitation and solution of the compound. Wagman (WA-901) and Rossini (RO-907) both base their values on J. Thomsen's data (TH-908) published in 1882-86. Wagman's value revises Rossini's, and agrees well with Gedansky's data. Gedansky's value was accepted.	-129.4
	-129.0	WA-901, WA-912 (TH-908)		
	-131.2	RO-907 (TH-908)		
Cu(OH)$_2$	-105.9	GE-902	Gedansky et al. (GE-902) recently measured by calorimetry the heat of solution of Cu(OH)$_{2(c)}$ in perchloric acid, and the heat of precipitation for the reaction $CuSO_4$ (dil.) + 2NaOH (dil.) = $Cu(OH)_2(c) + Na_2SO_4$ (dil.) The author seemed to have accounted fully for all possible errors. L. V. My (MY-901) determined the heat of reaction for the decomposition $Cu(OH)_{2(c)} = CuO_{(c)} + H_2O\ (g)$.	-105.9
	-107.64±2.0	ST-918 (MY-901)		
	-107.5	WA-901		
	-107.2	RO-907 (FR-914, TH-908, SA-918, DE-914, BO-914)		

COMPOUND	VALUE(KCAL/MOLE)	REFERENCE	REMARKS	ACCEPTED VALUE(KCAL/MOLE)
			Using reported heats of formation for CuO$_{(c)}$ and H$_2$O(g), $\Delta H°_f$ for Cu(OH)$_2$ was calculated. Wagman's sources are not known (WA-901). In an earlier NBS compilation, Rossini (RO-907) cites several references, but his value was not accepted because it was revised by Wagman's publication. Gedansky's value was accepted.	
N$_2$O$_3$(g)	+20.0	RO-907	Coughlin's value (CO-913) was derived from measured free energy data and estimated heat capacity and entropy data. This value was the only one not in good agreement with the other four. Hisatune's (HI-906) is calculated from spectroscopic and structural data. Stull (ST-906) recalculated ΔH_R to be 9.7 kcal/mole for the reaction. $N_2O_3 \rightleftarrows NO + NO_2$ from all the cited equilibrium measurements. Stull's value was accepted.	+19.8
	+17.5±4.5	CO-913 (AB-902)		
	+20.0	LA-908		
	+19.8	ST-906 (BE-923, AB-902, VE-905)		
	+20.0	HI-906		

TABLE II

CONFLICTING VALUES FOR THE ABSOLUTE ENTROPY OF INORGANIC COMPOUNDS

COMPOUND	VALUE (E.U.)	REFERENCE	REMARKS	ACCEPTED VALUE (E.U.)
Be_3N_2	8.157 8.17 12 12	ST-918 (JU-901) JU-901 ST-906 KE-911	The early JANAF value (ST-906) and Kelley's value (KE-911) are not acceptable because they are estimated. B. H. Justice (JU-901) measured the heat capacity of α-Be_3N_2 from 25-310°K by adiabatic calorimetry. Stull (ST-918) calculated the absolute entropy by integrating the data based on $S_{25} = 0.002$ e.u. The more recent JANAF value was adopted.	8.157
LiOH · H_2O	17.07 17.07±0.05 22.	LA-908 (BA-928) KE-912 (BA-928) RO-907	Rossini (RO-907) did not cite a reference for his reported entropy value. Therefore the original source could not be checked. Landolt-Boernstein (LA-908) and K. K. Kelley (KE-912) cited Bauer, Johnston, and Kerr's heat capacity data (BA-928), which yielded $S^\circ_{298.15} - S^\circ_{16.00} = 17.04$ and $S^\circ_{16.00} = 0.03$ (by extrapolation). The sum is 17.07±0.05 (KE-912).	17.07

TABLE II (cont'd.)

Page 2

COMPOUND	VALUE (E.U.)	REFERENCE	REMARKS	ACCEPTED VALUE (E.U.)
$Ca(OH)_2$	19.9±0.0 19.93 19.93±0.1 18.2	KU-903 (HA-936) LA-908 KE-912 RO-907	The value agreed upon by three of the four compilations was selected. This value was calculated from heat capacity data measured by Hatton and coworkers (HA-936).	19.9
$Mn(OH)_2$	23.7 21.1 21.1	WA-901, WA-912 (FO-903, NA-936) RO-907 LA-908 (RO-907)	Landolt-Boernstein (LA-908) references NBS Circular 500 (RO-907). An attempt was made to check the source, but no reference was given in the latter publication. Therefore Wagman's value (WA-901) was chosen. It was calculated from free energy data obtained from the solubility measurements of Fox et al. (FO-903) and R. Näsänen (NA-936).	23.7
$Co(OH)_2$	22.3 19.	GE-903 WA-901 (SI-901)	Wagman (WA-901) used the free energy data of Sillén (SI-901) to calculate the absolute entropy of $Co(OH)_{2(c)}$. Gedansky et al. (GE-903) derived their value from reported heats of formation of $Co(OH)_2$, Co^{+2}, and free	22.3

COMPOUND	VALUE (E.U.)	REFERENCE	REMARKS	ACCEPTED VALUE (E.U.)
			energy data. Since Gedansky's value for ΔH_f° for $Co(OH)_2$ was adopted, his entropy value was selected in order to keep the data base as internally consistent as possible.	
$Cd(OH)_2$	23.	WA-918	Landolt-Boernstein (LA-908) cites Rossini's value (RO-907) but Rossini does not give a reference. Kelley's value was eliminated because it was estimated. It is not known what source Wagman (WA-918) used, because the bibliography for his compilation has not yet been published. Wagman's value was selected.	23.
	22.8	LA-908 (RO-907)		
	22.8	RO-907		
	21.5±0.5	KE-912		

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CHEMICAL COMPOUND DATA FILE

AG
AGNO2
AGNO3
AGVO3
AG2AL2O4
AG2CO3
AG2CRO4
AG2CR2O4
AG2FE2O4
AG2MOO4
AG2O
AG2S
AG2SO3
AG2SO4
AG2TIO3
AG2WO4
AL
ALN
2 AL(NO2)3
AL(NO3)3
AL(NO3)3.6H2O
2 AL(NO3)3.9H2O
2 AL(OH)3
AL2O3
2 AL2S
AL2S3
AL2TIO5
AL2(CO3)3
AL2(CRO4)3
AL2(CR2O4)3
AL2(FE2O4)3
AL2(MOO4)3
AL2(SO3)3
AL2(SO4)3

AL2(TIO3)3
AL2(V2O6)3
AL2(WO4)3
AS
AS2O3
2 AS2O5
AS2S3
2 AS2S5
2 AS2(CO3)3
2 AS2(SO3)3
2 AS2(SO4)3
B
BA
BAAL2O4
BACO3
BACRO4
BACR2O4
BAFE2O4
2 BAMOO3
BAMOO4
BAO
BAS
BASO3
BASO4
BATIO3
BAV2O6
BAWO4
BA(NO2)2
2 BA(NO2)2.H2O
BA(NO3)2
2 BA(OH)2
2 BA(OH)2.H2O
2 BA(OH)2.8H2O
2 BA2TIO4

2 BA3N2
BE
BEAL2O4
BECO3
BECRO4
BECR2O4
BEFE2O4
BEMOO4
BEO
BES
BESO3
BESO4
BETIO3
BEV2O6
BEWO4
BE(NO2)2
BE(NO3)2
BE(OH)2
BE3N2
BI
2 BI(NO2)3
BI(NO3)3
2 BI(OH)3
BI2O3
BI2S3
BI2(AL2O4)3
BI2(CO3)3
BI2(CRO4)3
BI2(CR2O4)3
BI2(FE2O4)3
BI2(MOO4)3
BI2(SO3)3
BI2(SO4)3
BI2(TIO3)3

BI2(V2O6)3
BI2(WO4)3
2 BO(GAS)
BS(GAS)
B2O3
B2S3
C
CA
CAAL2O4
2 CAAL4O7
CACO3
CACRO4
CACR2O4
CAFE2O4
2 CAMOO3
CAMOO4
CAO
CAS
CASO3
CASO4
CATIO3
CAV2O6
CAWO4
CA(NO2)2
CA(NO3)2
2 CA(NO3)2.2H2O
2 CA(NO3)2.3H2O
2 CA(NO3)2.4H2O
CA(OH)2
CA2FE2O5
CA3N2
CD
CDAL2O4
CDCO3

1 INDICATES ADDITION OR REVISION
2 INDICATES INCOMPLETE DATA

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CHEMICAL COMPOUND DATA FILE

CDCRO4
CDCR2O4
CDFE2O4
CDMOO4
CDO
CDS
CDSO3
CDSO4
CDTIO3
CDV2O6
CDWO4
CD(NO2)2
CD(NO3)2
2 CD(NO3)2.2H2O
2 CD(NO3)2.4H2O
2 CD(OH)2
2 CD3N2
CE
2 CEN
CEO2
2 CES
CES2
2 CE(CO3)2
2 CE(NO2)3
2 CE(NO2)4
CE(NO3)3
CE(NO3)4
2 CE(SO3)2
CE(SO4)2
CE2O3
CE2S3
2 CE2(CO3)3
2 CE2(SO3)3
CE2(SO4)3

2 CE3S4
CO
COAL2O4
COCO3
COCRO4
COCR2O4
COFE2O4
COMOO4
2 COMPOUND
COO
COS
COSO3
COSO4
COTIO3
COV2O6
COWO4
CO(NO2)2
CO(NO3)2
2 CO(NO3)2.2H2O
2 CO(NO3)2.3H2O
2 CO(NO3)2.4H2O
2 CO(NO3)2.6H2O
2 CO(OH)2
2 CO(OH)3
CO2
2 CO2S3
2 CO3N
CO3O4
2 CO3S4
CR
CRN
CRO3
2 CR(NO2)3
2 CR(NO2)6

2 CR(NO3)3
2 CR(NO3)6
2 CR(OH)3
2 CR2N
CR2O3
2 CR2O7
2 CR2S3
2 CR2(CO3)3
2 CR2(SO3)3
2 CR2(SO4)3
CS
2 CSNO2
CSNO3
2 CSNO3.4H2O
2 CSOH
2 CSOH.H2O
CS2AL2O4
2 CS2CO3
CS2CRO4
CS2CRO4
CS2FE2O4
2 CS2MOO4
2 CS2O
2 CS2S
2 CS2SO3
CS2SO4
CS2TIO3
CS2V2O6
2 CS2WO4
CS2(G)
CU
CUAL2O4
CUCO3
CUCRO4

CUCR2O4
CUFEO2
CUFE2O4
CUMOO4
CUNO2
CUNO3
CUO
CUO*CUSO4
CUS
CUSO3
CUSO4
CUTIO3
CUVO3
CUV2O6
CUWO4
CU(NO2)2
CU(NO3)2
2 CU(NO3)2.3H2O
2 CU(NO3)2.6H2O
CU(OH)2
CU2AL2O4
CU2CO3
CU2CRO4
CU2CR2O4
CU2MOO4
CU2O
CU2S
CU2SO3
CU2SO4
CU2TIO3
CU2WO4
2 CU3N
C(O)
FE

1 INDICATES ADDITION OR REVISION
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     FEAL2O4               FE2(WO4)3               IR                    LA2S3
     FECO3                 FE3O4                   IRO2                2 LA2(CO3)3
     FECRO4                FE4N                    IRS2                2 LA2(SO3)3
     FECR2O4               GA                    2 IRS3                  LA2(SO4)3
     FEMOO4              2 GAN                   2 IR(SO4)2              LI
     FEO                 2 GAS                   2 IR2S3                 LIALO2
     FES                 2 GA(NO2)3                K                     LIFEO2
     FESO3               2 GA(NO3)3                KALO2                 LINO2
     FESO4               2 GA(OH)3                 KFEO2                 LINO3
     FES2                  GA2O3                   KNO2                2 LINO3.3H2O
     FETIO3                GA2S3                   KNO3                  LIOH
     FEV2O6              2 GA2(CO3)3               KOH                   LIOH.H2O
     FEWO4               2 GA2(SO3)3             2 KOH.H2O               LIVO3
     FE(NO2)2            2 GA2(SO4)3             2 KOH.0.75H2O           LI2CO3
   2 FE(NO2)3              GE                    2 KOH.2H2O              LI2CRO4
     FE(NO3)2            2 GEO(GAS)                KVO3                  LI2CR2O4
   2 FE(NO3)2.6H2O         GEO2                    K2CO3                 LI2MOO4
     FE(NO3)3              GES                     K2CRO4                LI2O
   2 FE(NO3)3.9H2O       2 GES2                    K2CR2O4               LI2S
   2 FE(OH)2             2 GE(CO3)2                K2MOO4                LI2SO3
     FE(OH)3             2 GE(SO3)2                K2O                   LI2SO4
     FE2N                2 GE(SO4)2                K2S                   LI2TIO3
     FE2O3               2 GE3N4                   K2SO3                 LI2WO4
   2 FE2TIO4               HF                      K2SO4                 LI3N
   2 FE2TIO5             2 HFN                     K2TIO3                MG
     FE2(AL2O4)3           HFO2                    K2WO4                 MGAL2O4
     FE2(CO3)3           2 HFS2                    LA                    MGCO3
     FE2(CRO4)3          2 HF(CO3)2              2 LAN                   MGCRO4
     FE2(CR2O4)3         2 HF(NO2)4              2 LAS                   MGCR2O4
     FE2(MOO4)3          2 HF(NO3)4              2 LAS2                  MGFE2O4
     FE2(SO3)3           2 HF(SO3)2              2 LA(NO2)3              MGMOO4
     FE2(SO4)3           2 HF(SO4)2                LA(NO3)3              MGO
     FE2(TIO3)3            H2                    2 LA(NO3)3.6H2O         MGS
     FE2(V2O6)3            H2O(GAS)                LA2O3                 MGSO3

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     MGSO4               2 MN(NO3)2.6H2O           NAALO2              2 NB2(SO3)5
     MGTIO3                MN(NO3)3                NACL                2 NB2(SO4)5
     MGTI2O5             2 MN(NO3)4                NAFEO2                NI
     MGV2O6              2 MN(OH)2                 NANO2                 NIAL2O4
     MGWO4               2 MN(OH)3                 NANO3                 NICO3
     MG(NO2)2            2 MN(SO4)2                NAOH                  NICRO4
     MG(NO3)2              MN2O3                 2 NAOH.H2O              NICR2O4
   2 MG(NO3)2.2H2O         MN2(AL2O4)3           2 NAOH.2H2O             NIFE2O4
   2 MG(NO3)2.6H2O         MN2(CO3)3             2 NAOH.3H2O             NIMOO4
     MG(OH)2               MN2(CRO4)3            2 NAOH.3.5H2O           NIO
   2 MG2TIO4               MN2(CR2O4)3           2 NAOH.4H2O             NIS
     MG3N2                 MN2(FE2O4)3           2 NAOH.5H2O             NISO3
     MN                    MN2(MOO4)3            2 NAOH.7H2O             NISO4
     MNAL2O4               MN2(SO3)3               NAVO3                 NITIO3
     MNCO3                 MN2(SO4)3               NA2CO3                NIV2O6
     MNCRO4                MN2(TIO3)3              NA2CRO4               NIWO4
     MNCR2O4               MN2(V2O6)3              NA2CR2O4              NI(NO2)2
     MNFE2O4               MN2(WO4)3               NA2MOO4               NI(NO3)2
     MNMOO4              2 MN3N2                   NA2MO2O7            2 NI(NO3)2.3H2O
     MNO                   MN3O4                   NA2O                2 NI(NO3)2.6H2O
     MNO2                  MN4N                    NA2S                2 NI(OH)2
     MNS                 2 MN5N2                   NA2SO3              2 NI(OH)3
     MNSO3               2 MN8N2                   NA2SO4              2 NI3N
     MNSO4                 MO                      NA2TIO3               NI3S2
     MNS2                2 MOO2                  2 NA2TI2O5              NO(G)
     MNTIO3                MOO3                  2 NA2TI3O7              NO2(G)
     MNV2O6                MOS2                    NA2WO4                N2O3(G)
     MNWO4                 MOS3                    NA2W2O7               N2O4(G)
     MN(NO2)2            2 MO(CO3)3                NB                    N2O5
   2 MN(NO2)3            2 MO(SO3)3              2 NBO                   N2O5(G)
   2 MN(NO2)4            2 MO(SO4)3              2 NBO2                  N2(GAS)
     MN(NO3)2              MO2N                    NB2O5                 O2
   2 MN(NO3)2.3H2O       2 MO2S3                 2 NB2S5                 PB
   2 MN(NO3)2.4H2O         NA                    2 NB2(CO3)5             PBAL2O4

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PBCO3
2 PBCO3*PBO
2 PBCO3*2PBO
PBCRO4
PBCR2O4
PBFE2O4
PBMOO4
PBO
PBO*PBSO4
PBO2
PBS
PBSO3
PBSO4
PBTIO3
PBV2O6
PBWO4
PB(NO2)2
2 PB(NO2)4
PB(NO3)2
2 PB(NO3)4
2 PB(OH)2
2 PB(SO4)2
2 PB3O4
PD
2 PDCO3
PDO
PDS
2 PDSO3
2 PDSO4
2 PDS2
2 RBNO2
RBNO3
2 RBOH
2 RBOH.H2O
2 RBOH.2H2O
RB2CO3
2 RB2O
2 RB2S
2 RB2SO3
2 RB2SO4
RE
2 REO2
2 REO3
2 RES2
2 RES3
2 RE2O7
2 RE2O8
2 RE2S7
RH
2 RHCO3
RHO
2 RHS
2 RHSO3
2 RHSO4
RH2O
RH2O3
2 RH2S
2 RH2SO4
2 RH2S3
2 RH2(SO4)3
RU
2 RUO2
2 RUO3(GAS)
2 RUO4(GAS)
2 RUS2
S
SB
SB2O3
SB2O4
2 SB2O5
SB2S3
SB2(AL2O4)3
SB2(CO3)3
SB2(CRO4)3
SB2(CR2O4)3
SB2(FE2O4)3
SB2(MOO4)3
SB2(SO3)3
SB2(SO4)3
SB2(TIO3)3
SB2(V2O6)3
SB2(WO4)3
SC
SC2O3
2 SC2(CO3)3
2 SC2(SO3)3
2 SC2(SO4)3
SI
2 SIO(GAS)
SIO2
SIS(GAS)
SIS2
2 SI(CO3)2
2 SI(SO3)2
2 SI(SO4)2
SN
2 SNCO3
SNO
SNO2
SNS
2 SNSO3
2 SNSO4
SNS2
SN(AL2O4)2
SN(CO3)2
SN(CRO4)2
SN(CR2O4)2
SN(FE2O4)2
SN(MOO4)2
2 SN(NO2)2
2 SN(NO2)4
2 SN(NO3)2
SN(NO3)4
2 SN(OH)2
2 SN(OH)4
SN(SO3)2
SN(SO4)2
SN(TIO3)2
SN(V2O6)2
SN(WO4)2
SO2
SO3
SR
SRAL2O4
SRCO3
SRCRO4
SRCR2O4
SRFE2O4
2 SRMOO3
SRMOO4
SRO
SRS
SRSO3
SRSO4
SRTIO3
SRV2O6

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SRWO4
SR(NO2)2
SR(NO3)2
2 SR(NO3)2.4H2O
2 SR(OH)2
2 SR(OH)2.H2O
2 SR(OH)2.8H2O
2 SR2TIO4
2 SR3N2
S(GAS)
TA
TAN
2 TA2N
TA2O5
2 TA2S5
2 TA2(CO3)5
2 TA2(SO3)5
2 TA2(SO4)5
TH
THO2
2 THS
THS2
TH(AL2O4)2
TH(CO3)2
TH(CRO4)2
TH(CR2O4)2
TH(FE2O4)2
TH(MOO4)2
TH(SO3)2
TH(SO4)2
TH(TIO3)2
TH(V2O6)2
TH(WO4)2
TH2S3
TI
2 TICO3
TIN
TIO
TIO2
2 TISO3
2 TISO4
TIS2
2 TI(NO2)2
2 TI(NO2)3
2 TI(NO2)4
2 TI(NO3)2
2 TI(NO3)3
2 TI(NO3)4
2 TI(SO4)2
TI2O3
2 TI2(CO3)3
2 TI2(SO3)3
2 TI2(SO4)3
TI3O5
U
UO2
UO2SO4
UO3
2 US
US2
U(AL2O4)2
U(CO3)2
U(CRO4)2
U(CR2O4)2
U(FE2O4)2
U(MOO4)2
U(SO3)2
U(SO4)2
U(TIO3)2
U(V2O6)2
U(WO4)2
2 U2S3
U3O8
V
2 VCO3
2 VN
VO
VOSO4
VS
2 VSO3
2 VSO4
V2O3
V2O4
V2O5
2 V2S3
2 V2S4
2 V2S5
2 V2(CO3)3
2 V2(SO3)3
2 V2(SO4)3
W
WO2
WO3
WS2
2 W(CO3)2
2 W(CO3)3
2 W(SO3)2
2 W(SO3)3
2 W(SO4)2
2 W(SO4)3
Y
Y2O3
2 Y2(CO3)3
2 Y2(SO3)3
2 Y2(SO4)3
ZN
ZNAL2O4
ZNCO3
ZNCRO4
ZNCR2O4
ZNFE2O4
ZNMOO4
ZNO
ZNO*2ZNSO4
ZNS
ZNSO3
ZNSO4
ZNTIO3
ZNV2O6
ZNWO4
ZN(NO2)2
ZN(NO3)2
2 ZN(NO3)2.H2O
2 ZN(NO3)2.2H2O
2 ZN(NO3)2.4H2O
2 ZN(NO3)2.6H2O
2 ZN(OH)2
ZN2TIO4
2 ZN3N2
ZR
ZRN
ZRO2
2 ZRS2
ZR(AL2O4)2
ZR(CO3)2
ZR(CRO4)2

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ZR(CR2O4)2
ZR(FE2O4)2
ZR(MOO4)2
2 ZR(NO2)2
2 ZR(NO2)4
2 ZR(NO3)2
2 ZR(NO3)2.6H2O
ZR(NO3)4
2 ZR(OH)4
2 ZR(OH)4.H2O
2 ZR(OH)4.2H2O
ZR(SO3)2
ZR(SO4)2
ZR(TIO3)2
ZR(V2O6)2
ZR(WO4)2
2 ZR3N2

1 INDICATES ADDITION OR REVISION
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TABLE V

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HEAT OF FORMATION, ENTROPY, AND TRANSITION DATA

COMPOUND	HEAT OF FORMATION 25 DEG.C KCAL/GMOLE	REFERENCES	ABSOLUTE ENTROPY CAL/GMOLE/ DEG. K	REFERENCES	TRANSITION DATA			
					TEMP. DEG.C	HEAT KCAL/ GMOLE	TYPE	REFERENCES
AG	.00		10.20	LA-001	961.28	2.69	S-L	LA-001
AGNO2	-10.77	WA-901,ST-926	30.64	WA-901,ST-926				
AGNO3	-29.73	WA-901	33.68	WA-901,RO-907	160.00	.66	S-S	RO-907
					210.00	2.76	S-L	
AGVO3	-199.53	TR-002	32.60	KE-001				
AG2AL2O4	-413.64	TR-002	44.20	TR-003				
AG2CO3	-120.88	LA-001	39.97	LA-001				
AG2CRO4	-172.37	CA-058	52.00	CA-058				
AG2CR2O4	-308.20	TR-002	49.60	KE-001				
AG2FE2O4	-205.53	TR-002	51.26	TR-003				
AG2MOO4	-216.60	CA-056	61.86	CA-058				
AG2O	-7.30	LA-001	29.07	LA-001				
AG2S	-7.75	LA-001,NB-003	34.00	LA-001,KU-001	179.00	1.05	S-S	LA-001
					582.00		S-S	
					842.00	3.36	S-L	
AG2SO3	-114.40	CA-006	44.60	TR-003				
AG2SO4	-170.36	LA-001	47.76	LA-001	441.00	4.46	S-S	LA-001,CA-002
					657.00	4.28	S-L	
AG2TIO3	-239.37	TR-002	40.10	TR-003				
AG2WO4	-230.70	HE-001	27.16	CA-058				
AL	.00		6.76	LA-001	658.60	2.56	S-L	LA-001
ALN	-76.00	ST-906,RA-001	4.82	ST-906	2227.00		S-L	LA-908
AL(NO2)3	-190.82	RA-002						
AL(NO3)3	-239.38	RA-002	53.00	RA-004				
AL(NO3)3.6H2O	-681.30	WA-918	111.80	LA-908,KE-912				
AL(NO3)3.9H2O	-897.96	WA-918	136.00	LA-908,RO-907				
AL(OH)3	-304.20	RO-907						
AL2O3	-400.16	LA-001,NB-002	12.17	LA-001,NB-002	975.00	20.59	S-S	LA-001
					2045.00	26.04	S-L	
					3530.00		L-G	
AL2S	-29.38	LA-001	73.10	LA-001				
AL2S3	-172.85	LA-001,TR-010	23.00	LA-001,NB-003	1100.00		S-L	LA-001

DATE 6 OCT. 1971 HEAT OF FORMATION, ENTROPY, AND TRANSITION DATA (CONTINUED) PAGE: 2

COMPOUND	HEAT OF FORMATION 25 DEG.C KCAL/GMOLE	REFERENCES	ABSOLUTE ENTROPY CAL/GMOLE/ DEG. K	REFERENCES	TRANSITION DATA			
					TEMP. DEG.C	HEAT KCAL/ GMOLE	TYPE	REFERENCES
AL2TIO5	-622.96	CA-043	26.20	KU-001	1890.00		S-L	KU-001
AL2(CO3)3	-707.03	TR-002	40.00	TR-003				
AL2(CRO4)3	-849.81	TR-002	78.60	KE-001				
AL2(CR2O4)3	-1238.00	TR-002	68.40	KE-001				
AL2(FE2O4)3	-975.13	TR-002	75.60	KE-001				
AL2(MOO4)3	-979.92	TR-002	64.60	TR-007				
AL2(SO3)3	-661.91	TR-002	49.00	TR-003				
AL2(SO4)3	-820.38	LA-001,NB-003	57.14	LA-001,NB-003				
AL2(TIO3)3	-1074.60	TR-002	42.60	KE-001				
AL2(V2O6)3	-1532.00	TR-002	115.20	KE-001				
AL2(WO4)3	-1023.70	TR-002	62.20	TR-007				
AS	.00		8.39	LA-001				
AS2O3	-156.91	LA-001,KU-001	25.59	LA-001,KU-001	274.00	11.90	S-S	
					315.00	4.47	S-S	
AS2O5	-219.31	LA-001	25.18	LA-001				
AS2S3	-30.00	KU-001,TR-010	27.71	TR-003	170.00		S-S	
					300.00		S-L	
AS2S5	-35.00	KU-001	44.20	KE-001	170.00		S-S	KU-001
					300.00		S-L	
AS2(CO3)3			46.90	TR-003				
AS2(SO3)3			55.90	TR-003				
AS2(SO4)3			64.00	TR-003				
B	.00		1.40	LA-001	2030.00	5.30	S-L	LA-001
BA	.00		15.49	LA-001	370.00	.14	S-S	LA-001
					710.00	1.83	S-L	
BAAL2O4	-566.67	TR-002	28.58	TR-003				
BACO3	-287.16	LA-001	26.78	LA-001	806.00	3.87	S-S	LA-001
					968.00	.69	S-S	
BACRO4	-336.37	TR-002	38.15	TR-003				
BACR2O4	-516.32	TR-002	33.22	TR-003				
BAFE2O4	-350.49	CA-061	35.37	TR-003				
BAMOO3	-308.70	CA-024						
BAMOO4	-377.04	TR-002	33.97	TR-003				

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 COMPOUND          HEAT  OF    REFERENCES      ABSOLUTE     REFERENCES                         TRANSITION DATA
                   FORMATION                   ENTROPY                           TEMP.     HEAT   TYPE   REFERENCES
                   25 DEG.C                   CAL/GMOLE/                         DEG.C     KCAL/
                  KCAL/GMOLE                   DEG. K                                      GMOLE


BAO                 -132.07   LA-001,CA-007      16.79   LA-001              1923.00     13.78   S-L   LA-001
                                                                             2700.00             L-G
BAS                 -106.00   CA-019,TR-010      20.90   LA-001,TR-010
BASO3               -282.60   NB-003             28.60   TR-003
BASO4               -349.99   LA-001             31.49   LA-001              1150.00             S-S   LA-001,CA-002
                                                                             1350.00      9.70   S-L
BATIO3              -394.60   CA-063,TR-002      25.78   LA-001
BAV2O6              -567.34   TR-002             45.78   TR-003
BAWO4               -406.00   CA-025             32.00   CA-025
BA(NO2)2            -183.60   ST-926,RA-001      43.70   RA-004               273.00             S-L   ST-926
BA(NO2)2.H2O        -254.50   RO-907
BA(NO3)2            -237.11   ST-926             51.10   ST-926,KE-912        595.00      6.00   S-L   LA-908,RO-907
BA(OH)2             -226.10   LA-908                                          246.00             S-S   MI-907
                                                                              408.00      3.72   S-L
BA(OH)2.H2O         -299.00   RO-907
BA(OH)2.8H2O        -799.50   RO-907
BA2TIO4                                          47.00   KU-001
BA3N2                -86.90   KU-903,RA-001      36.30   LA-908
BE                      .00                       2.27   LA-001              1283.00      2.99   S-L   LA-001
BEAL2O4             -542.99   TR-002,CA-065      19.18   TR-003
BECO3               -246.39   TR-002             15.69   TR-003
BECRO4              -294.44   TR-002             28.75   TR-003
BECR2O4             -424.43   TR-002             23.82   TR-003
BEFE2O4             -335.85   TR-002             25.97   TR-003
BEMOO4              -337.96   TR-002             24.57   TR-003
BEO                 -143.03   LA-001              3.37   LA-001              2550.00     16.99   S-L   LA-001
                                                                             4120.00             L-G
BES                  -55.90   KU-001,NB-003       8.40   KU-001,LA-001
BESO3               -232.20   TR-002             19.20   TR-003
BESO4               -285.65   NB-003             18.62   CA-005               880.00      3.30   S-S   CA-005
BETIO3              -368.42   TR-002             17.21   TR-003
BEV2O6              -521.71   TR-002             36.38   TR-003
BEWO4               -352.45   TR-002             23.56   TR-003
BE(NO2)2            -138.65   RA-002             34.30   RA-004
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 COMPOUND          HEAT  OF    REFERENCES      ABSOLUTE     REFERENCES                         TRANSITION DATA
                   FORMATION                   ENTROPY                           TEMP.     HEAT   TYPE   REFERENCES
                   25 DEG.C                   CAL/GMOLE/                         DEG.C     KCAL/
                  KCAL/GMOLE                   DEG. K                                      GMOLE


BE(NO3)2            -171.71   RA-002             39.60   RA-003
BE(OH)2             -215.75   ST-918             11.80   ST-918
BE3N2               -140.60   ST-918,RA-001       8.16   ST-918,RA-001       2200.00     30.90   S-L   ST-918
BI                      .00                      13.56   LA-001               271.30      2.60   S-L   LA-001
BI(NO2)3             -78.17   RA-002
BI(NO3)3            -133.21   RA-002             60.60   RA-004
BI(OH)3             -170.00   WA-918
BI2O3               -138.98   LA-001,NB-001      36.12   LA-001,NB-001        704.00             S-S   LA-001
                                                                              817.00      6.81   S-L
BI2S3                -43.80   NB-003,WI-001      35.30   NB-003
BI2(AL2O4)3        -1549.50   TR-002             78.20   KE-001
BI2(CO3)3           -476.57   TR-002             55.20   TR-003
BI2(CRO4)3          -618.62   TR-002            106.40   KE-001
BI2(CR2O4)3        -1024.00   TR-002             96.20   KE-001
BI2(FE2O4)3         -727.92   TR-002            106.40   KE-001
BI2(MOO4)3          -749.96   TR-002             79.80   TR-007
BI2(SO3)3           -437.25   TR-002             64.20   TR-003
BI2(SO4)3           -608.10   NB-001,WI-001      72.30   TR-003
BI2(TIO3)3          -826.08   TR-002             70.40   KE-001
BI2(V2O6)3         -1300.00   TR-002            143.00   KE-001
BI2(WO4)3           -794.59   TR-002             77.40   TR-007
BO(GAS)               -5.30   LA-001             48.59   LA-001
BS(GAS)              -80.00   JA-001             51.65   JA-001
B2O3                -306.10   KU-001,TR-010      12.86   LA-001               450.00      5.49   S-L   LA-001
B2S3                 -57.00   LA-001,NB-003      14.61   TR-003               310.00             S-L   LA-001,KU-001
C                       .00   JA-001              1.36   JA-001
CA                      .00                       9.94   LA-001               440.00       .24   S-S   LA-001
                                                                              850.00      2.07   S-L
CAAL2O4             -555.50   KU-001             27.30   KU-001
CAAL4O7                                          42.50   KU-001
CACO3               -288.11   LA-001             22.19   LA-001
CACRO4              -329.44   LA-001             32.01   LA-001
CACR2O4             -492.40   CA-038             28.82   TR-003
CAFE2O4             -367.25   CA-042,TR-010      34.70   KU-001,LA-001       1240.00     25.85   S-L   KU-001
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DATE 6 OCT. 1971 HEAT OF FORMATION, ENTROPY, AND TRANSITION DATA (CONTINUED) PAGE: 5

COMPOUND	HEAT OF FORMATION 25 DEG.C KCAL/GMOLE	REFERENCES	ABSOLUTE ENTROPY CAL/GMOLE/ DEG. K	REFERENCES	TRANSITION DATA			
					TEMP. DEG.C	HEAT KCAL/ GMOLE	TYPE	REFERENCES
CAMOO3	-277.80	CA-020	24.70	CA-021				
CAMOO4	-369.21	CA-077,TR-010	29.30	KU-001,CA-017				
CAO	-151.73	LA-001,NB-003	9.48	NB-003,LA-001	2603.00	12.23	S-L	LA-001
					3570.00		L-G	
CAS	-114.20	LA-001,TR-010	13.50	KU-001,NB-003				
CASO3	-275.88	MA-001	24.20	LA-001				
CASO4	-340.19	LA-001	25.49	LA-001	1193.00		S-S	LA-001,CA-002
					1397.00	6.69	S-L	
CATIO3	-370.00	CA-053	22.40	KU-001,TR-010	1260.00	.55	S-S	KU-001,LA-001
CAV2O6	-556.70	CA-050	42.60	CA-052				
CAWO4	-402.50	CA-077,TR-010	30.20	KU-001,TR-010				
CA(NO2)2	-177.20	ST-926,RA-001	39.30	RA-004	266.00		S-S	ST-926
					360.00		S-S	
					392.00		S-L	
CA(NO3)2	-224.28	ST-926	46.20	LA-908,ST-926	561.00	5.09	S-L	LA-908
CA(NO3)2.2H20	-367.80	LA-908	64.30	LA-908				
CA(NO3)2.3H20	-436.90	LA-908	74.10	LA-908	51.10		S-L	LA-908,RO-907
CA(NO3)2.4H20	-509.10	LA-908	61.00	LA-908,RO-907	39.70		S-L	LA-908,RO-907
CA(OH)2	-237.50	KU-903,RA-001	19.93	LA-908,RA-001				
CA2FE2O5	-507.28	KU-001	45.10	KU-001				
CA3N2	-104.30	LA-908	25.10	LA-908	1195.00		S-L	LA-908,KU-903,
CD	.00		12.37	LA-001	321.00	1.53	S-L	LA-001
CDAL2O4	-466.54	TR-002	27.76	TR-003				
CDCO3	-178.46	LA-001	25.18	LA-001				
CDCRO4	-224.10	TR-002	37.35	TR-003				
CDCR2O4	-361.66	TR-002	32.42	TR-003				
CDFE2O4	-258.73	TR-002	34.57	TR-003				
CDMOO4	-267.85	TR-002	33.17	TR-003				
CDO	-61.18	LA-001	13.09	LA-001				
CDS	-34.47	LA-001,NB-003	16.96	LA-001,NB-003				
CDSO3	-163.90	CA-001	27.80	TR-003				
CDSO4	-221.20	LA-001	29.41	LA-001	792.00	1.49	S-S	LA-001,CA-002
					859.00	2.39	S-S	
					1000.00		S-L	

DATE 6 OCT. 1971 HEAT OF FORMATION, ENTROPY, AND TRANSITION DATA (CONTINUED) PAGE: 6

COMPOUND	HEAT OF FORMATION 25 DEG.C KCAL/GMOLE	REFERENCES	ABSOLUTE ENTROPY CAL/GMOLE/ DEG. K	REFERENCES	TRANSITION DATA			
					TEMP. DEG.C	HEAT KCAL/ GMOLE	TYPE	REFERENCES
CDTIO3	-292.23	TR-002	25.80	TR-003				
CDV2O6	-451.32	TR-002	44.98	TR-003				
CDWO4	-283.05	TR-002,WI-001	32.16	TR-003				
CD(NO2)2	-70.77	RA-002	42.90	RA-004				
CD(NO3)2	-109.06	ST-926,WA-918	48.20	RA-003	360.00	4.35	S-L	ST-926
CD(NO3)2.2H20	-252.30	WA-918						
CD(NO3)2.4H20	-394.11	WA-918			59.50	7.80	S-L	RO-907
CD(OH)2	-134.00	WA-918	23.00	WA-918,RA-001				
CD3N2	38.60	KU-903,RO-907						
CE	.00		16.63	LA-001	393.00		S-S	LA-001
					440.00		S-S	
					777.00	3.08	S-L	
CEN	-77.90	LA-908						
CEO2	-233.00	LA-001,NB-003	14.89	CA-066				
CES	-118.00	KU-001	18.30	TR-003				
CES2	-153.90	NB-003	18.82	TR-003				
CE(CO3)2	-468.01	TR-002						
CE(NO2)3	-245.73	RA-002						
CE(NO2)4	-255.88	RA-002						
CE(NO3)3	-306.68	RA-002	58.80	RA-004				
CE(NO3)4	-332.66	RA-002	69.80	RA-004				
CE(SO3)2	-443.14	TR-002						
CE(SO4)2	-560.00	NB-003,WI-001	37.80	TR-003				
CE2O3	-434.90	KU-001,CA-018	36.00	CA-014,TR-010				
CE2S3	-298.70	NB-003,KU-001	32.41	TR-003	1890.00		S-L	KU-001
CE2(CO3)3			51.60	TR-003				
CE2(SO3)3			60.60	TR-003				
CE2(SO4)3	-953.00	MA-001	68.70	TR-003				
CE3S4	-421.50	KU-001			2050.00		S-L	KU-001
CO	.00		7.18	LA-001	445.00	.00	S-S	LA-001
					1127.00	.13	S-S	
					1490.00	3.66	S-L	
COAL2O4	-466.50	CA-055	25.48	TR-003				
COCO3	-173.30	KE-002	21.99	TR-003				

COMPOUND	HEAT OF FORMATION 25 DEG.C KCAL/GMOLE	REFERENCES	ABSOLUTE ENTROPY CAL/GMOLE/ DEG. K	REFERENCES	TRANSITION DATA			
					TEMP. DEG.C	HEAT KCAL/ GMOLE	TYPE	REFERENCES
COCRO4	-221.49	TR-002	35.05	TR-003				
COCR2O4	-350.60	CA-034	27.00	CA-034				
COFE2O4	-255.26	TR-002	32.20	KU-001,TR-003	500.00		S-S	CA-056
COMOO4	-265.21	TR-002	30.87	TR-003				
COMPOUND	.00							
COO	-57.07	LA-001	12.65	LA-001	1800.00	9.60	S-L	LA-001
COS	-21.07	RO-004,TR-010	15.82	TR-003	1100.00		S-L	LA-001
COSO3	-161.75	TR-002	25.50	TR-003				
COSO4	-211.90	AU-001,TR-010	27.07	LA-001	691.00	.51	S-S	CA-002
COTIO3	-289.50	CA-033,CA-055	23.80	CA-033				
COV2O6	-448.77	TR-002	42.66	TR-003				
COWO4	-280.61	TR-002	29.96	TR-003				
CO(NO2)2	-63.40	RA-002	40.60	RA-004				
CO(NO3)2	-100.50	WA-901,RA-001	45.90	RA-003				
CO(NO3)2.2H2O	-244.20	WA-901						
CO(NO3)2.3H2O	-316.90	WA-901			91.00		S-L	RO-907
CO(NO3)2.4H2O	-389.70	WA-901						
CO(NO3)2.6H2O	-528.49	WA-901			-33.00	1.70	S-S	RO-907,PO-912
					20.00	.70	S-S	
					57.00		S-L	
CO(OH)2	-129.40	GE-903,RA-001	22.30	GE-903,RA-001				
CO(OH)3	-171.30	WA-901						
CO2	-94.01	LA-001	51.03	LA-001				
CO2S3	-51.00	NB-003	26.40	TR-003				
CO3N	2.00	KU-903						
CO3O4	-216.20	LA-001	24.61	LA-001				
CO3S4	-75.00	KU-001						
CR	.00		5.68	LA-001	1840.00	.35	S-S	LA-001
					1903.00	3.49	S-L	
CRN	-29.80	WA-901,KE-911	7.85	KU-903				
CRO3	-142.03	LA-001	17.20	LA-001	187.00		S-L	
CR(NO2)3								
CR(NO2)6								
CR(NO3)3			55.20	RA-004				

COMPOUND	HEAT OF FORMATION 25 DEG.C KCAL/GMOLE	REFERENCES	ABSOLUTE ENTROPY CAL/GMOLE/ DEG. K	REFERENCES	TRANSITION DATA			
					TEMP. DEG.C	HEAT KCAL/ GMOLE	TYPE	REFERENCES
CR(NO3)6								
CR(OH)3	-254.30	WA-901						
CR2N	-30.50	WA-901,RA-001						
CR2O3	-272.58	LA-001	19.37	LA-001	32.80		S-S	LA-001
					2440.00		S-L	
CR2O7	-344.97	LA-001	70.48	LA-001				
CR2S3			25.21	TR-003				
CR2(CO3)3			44.40	TR-003				
CR2(SO3)3			53.40	TR-003				
CR2(SO4)3			61.50	TR-003				
CS	.00		20.14	LA-001	28.64	.52	S-L	LA-001
CSNO2	-88.69	RA-002	31.44	RA-003	406.00		S-L	ST-926
CSNO3	-121.80	ST-926	35.08	RA-003	151.50	.89	S-S	PO-912
					405.50	3.37	S-L	
CSNO3.4H2O					42.70		S-L	RO-907
CSOH	-97.15	LA-908			223.00	1.76	S-S	LA-908,RO-907
					272.50	1.61	S-L	
CSOH.H2O	-186.90	RO-907						
CS2AL2O4	-539.18	TR-002	45.80	TR-003				
CS2CO3	-272.57	TR-002	43.23	TR-003	792.00		S-L	HE-001
CS2CRO4	-318.00	TR-002	58.40	KE-001				
CS2CRO4	-551.92	TR-002	55.00	KE-001				
CS2FE2O4	-327.16	TR-002	52.86	TR-003				
CS2MOO4	-354.07	TR-002						
CS2O	-76.00	LA-001,CO-001	29.90	TR-003,CO-001	490.00	4.58	S-L	CO-001
CS2S	-81.10	NB-003,KU-001	35.14	TR-003				
CS2SO3	-265.60	CA-080	46.20	TR-003				
CS2SO4	-339.00	LA-001	50.89	TR-003	660.00		S-S	LA-001,CA-002
					722.00	.50	S-S	
					1004.00	9.52	S-L	
CS2TIO3	-368.44	TR-002	31.70	TR-003				
CS2V2O6	-554.30	TR-002	70.24	KE-001				
CS2WO4	-391.00	TR-002						
CS2(G)	27.55	LA-001	56.81	LA-001				

DATE 6 OCT. 1971 HEAT OF FORMATION, ENTROPY, AND TRANSITION DATA (CONTINUED) PAGE: 9

COMPOUND	HEAT OF FORMATION 25 DEG.C KCAL/GMOLE	REFERENCES	ABSOLUTE ENTROPY CAL/GMOLE/ DEG. K	REFERENCES	TRANSITION DATA			
					TEMP. DEG.C	HEAT KCAL/ GMOLE	TYPE	REFERENCES
CU	.00		7.96	LA-001	1084.00	3.11	S-L	LA-001
CUAL2O4	-439.03	TR-002	25.68	TR-003				
CUCO3	-142.10	LA-001	21.02	LA-001				
CUCRO4	-189.80	TR-002	35.25	TR-003				
CUCR2O4	-321.74	TR-002	30.32	TR-003				
CUFEO2	-115.90	TR-002	21.20	CA-062	1197.00	15.38	S-L	CA-062
CUFE2O4	-237.51	CA-042	32.47	TR-003				
CUMOO4	-233.21	TR-002	31.07	TR-003				
CUNO2	-16.84	RA-002	28.64	RA-003				
CUNO3	-32.84	RA-002	32.28	RA-003				
CUO	-37.25	ST-918	10.19	LA-001				
CUO*CUSO4	-222.35	IN-001	38.03	IN-001				
CUS	-11.50	LA-001,KU-001	15.90	LA-001,KU-001				
CUSO3	-127.28	TR-002	25.70	TR-003				
CUSO4	-184.22	LA-001	27.07	LA-001				
CUTIO3	-264.49	TR-002	23.71	TR-003				
CUVO3	-208.68	TR-002	29.60	KE-001				
CUV2O6	-417.15	TR-002	42.88	TR-003				
CUWO4	-247.76	TR-002,WI-001	30.06	TR-003				
CU(NO2)2	-36.70	RA-002	40.80	RA-004				
CU(NO3)2	-72.40	WA-901,ST-926	46.10	RA-003	255.00		S-L	ST-926
CU(NO3)2,3H2O	-290.90	WA-901						
CU(NO3)2,6H2O	-504.50	WA-901			24.40	8.70	S-L	LA-908
CU(OH)2	-105.90	GE-902,RA-001	20.70	GE-902				
CU2AL2O4	-439.71	TR-002	40.20	TR-003				
CU2CO3	-142.29	TR-002	37.63	TR-003				
CU2CRO4	-189.90	TR-002	47.00	KE-001				
CU2CR2O4	-319.04	TR-002	43.60	KE-001				
CU2MOO4	-233.18	TR-002	46.75	TR-007				
CU2O	-40.78	LA-001	22.52	LA-001	1230.00	13.38	S-L	LA-001
CU2S	-19.93	LA-001,NB-003	28.88	LA-001,NB-003	103.00	1.34	S-S	LA-001,KU-001
					350.00	.20	S-S	
					1127.00	5.49	S-L	
CU2SO3	-127.06	TR-002	40.60	TR-003				

DATE 6 OCT. 1971 HEAT OF FORMATION, ENTROPY, AND TRANSITION DATA (CONTINUED) PAGE: 10

COMPOUND	HEAT OF FORMATION 25 DEG.C KCAL/GMOLE	REFERENCES	ABSOLUTE ENTROPY CAL/GMOLE/ DEG. K	REFERENCES	TRANSITION DATA			
					TEMP. DEG.C	HEAT KCAL/ GMOLE	TYPE	REFERENCES
CU2SO4	-179.51	LA-001	38.46	LA-001				
CU2TIO3	-265.20	TR-002	36.10	TR-003				
CU2WO4	-247.85	TR-002	45.70	TR-007				
CU3N	17.80	WA-901,LA-908						
C(O)	-26.40	LA-001	47.16	LA-001				
FE	.00		6.49	LA-001	760.00	.00	S-S	LA-001
					906.00	.21	S-S	
					1401.00	.11	S-S	
					1535.00	3.70	S-L	
FEAL2O4	-474.40	CA-032,CA-054	25.40	KU-001				
FECO3	-178.55	LA-001	22.19	LA-001				
FECRO4	-225.69	TR-002	34.85	TR-003				
FECR2O4	-349.50	CA-068,TR-010	34.90	LA-001,KU-001	2180.00		S-L	LA-001,KU-001
FEMOO4	-269.45	TR-002	30.90	CA-064				
FEO	-63.76	LA-001	14.19	LA-001	-84.70		S-S	LA-001
					1377.00	7.48	S-L	
FES	-22.80	KU-001,LA-001	15.20	KU-001,LA-001	138.00	.57	S-S	KU-001,LA-001
					325.00	.12	S-S	
					1195.00	7.73	S-L	
FESO3	-165.54	TR-002	25.30	TR-003				
FESO4	-220.41	LA-001	25.68	LA-001				
FES2	-42.45	LA-001,KU-001	12.70	LA-001,KU-001				
FETIO3	-295.10	LA-001,TR-010	25.30	LA-001,KU-001	1370.00	21.70	S-L	LA-001,KU-001
FEV2O6	-452.87	TR-002	42.48	TR-003				
FEWO4	-284.52	TR-002	31.50	CA-064				
FE(NO2)2	-70.36	RA-002	40.40	RA-004				
FE(NO2)3	-88.59	RA-002						
FE(NO3)2	-107.23	RA-002	45.70	RA-003				
FE(NO3)2,6H2O					60.50		S-L	RO-907
FE(NO3)3	-137.01	RA-002	55.40	RA-004				
FE(NO3)3,9H2O	-785.20	WA-901,RA-001			50.10		S-L	LA-908,RO-907
FE(OH)2	-137.20	ST-918,RA-001						
FE(OH)3	-196.70	WA-901	25.50	WA-901				
FE2N	-.90	LA-908,KU-903	24.20	LA-908,KU-903				

COMPOUND	HEAT OF FORMATION 25 DEG.C KCAL/GMOLE	REFERENCES	ABSOLUTE ENTROPY CAL/GMOLE/DEG. K	REFERENCES	TRANSITION DATA			
					TEMP. DEG.C	HEAT KCAL/GMOLE	TYPE	REFERENCES
FE2O3	-196.42	LA-001	20.88	LA-001	677.00 767.00	.16	S-S S-S	LA-001
FE2TIO4			39.00	KU-001				
FE2TIO5			37.40	KU-001				
FE2(AL2O4)3	-1349.30	TR-002	61.60	KE-001				
FE2(CO3)3	-502.66	TR-002	44.80	TR-003				
FE2(CRO4)3	-645.46	TR-002	89.80	KE-001				
FE2(CR2O4)3	-1033.40	TR-002	79.60	KE-001				
FE2(MOO4)3	-775.50	TR-002	69.40	TR-007				
FE2(SO3)3	-457.40	TR-002	53.80	TR-003				
FE2(SO4)3	-615.80	CA-009	61.90	TR-003				
FE2(TIO3)3	-870.56	TR-002	53.80	KE-001				
FE2(V2O6)3	-1327.70	TR-002	126.40	KE-001				
FE2(WO4)3	-819.32	TR-002	67.00	TR-007				
FE3O4	-266.61	LA-001	34.97	LA-001	627.00 1594.00	 32.97	S-S S-L	LA-001
FE4N	-2.50	WA-901	37.00	WA-901				
GA	.00		9.82	LA-001	29.78	1.33	S-L	LA-001
GAN	-26.40	WA-918	11.00	LA-908,KU-903				
GAS	-46.40	LA-001,KU-001	16.22	TR-003	965.00		S-L	LA-001,NB-003
GA(NO2)3								
GA(NO3)3			56.20	RA-004				
GA(OH)3	-230.50	WA-918	24.00	WA-918				
GA2O3	-261.05	WA-003,TR-010	20.22	LA-001,NB-002	1725.00		S-L	LA-001
GA2S3	-136.80	KU-001	27.21	TR-003				
GA2(CO3)3			46.40	TR-003				
GA2(SO3)3			55.40	TR-003				
GA2(SO4)3			63.50	TR-003				
GE	.00		7.43	LA-001	937.20	7.12	S-L	LA-001
GEO(GAS)	-22.79	LA-001	52.51	LA-001				
GEO2	-129.15	LA-001	13.20	LA-001	707.00 1115.00	42.05 10.49	S-S S-L	LA-001
GES	-21.40	KU-001,TR-010	15.77	CA-084,KU-001	625.00 760.00	5.97	S-L L-G	LA-001,CA-072, KU-001

DATE 6 OCT. 1971 HEAT OF FORMATION, ENTROPY, AND TRANSITION DATA (CONTINUED) PAGE: 12

COMPOUND	HEAT OF FORMATION 25 DEG.C KCAL/GMOLE	REFERENCES	ABSOLUTE ENTROPY CAL/GMOLE/DEG. K	REFERENCES	TRANSITION DATA			
					TEMP. DEG.C	HEAT KCAL/GMOLE	TYPE	REFERENCES
GES2			19.00	CA-072	825.00	10.00	S-L	CA-072
GE(CO3)2			34.20	KE-001				
GE(SO3)2			45.20	KE-001				
GE(SO4)2			35.30	TR-003				
GE3N4	-15.60	LA-908,KU-903	40.00	KU-903,LA-908				
HF	.00		10.91	LA-001	1550.00 2222.00	 5.21	S-S S-L	LA-001
HFN	-88.24	LA-908,KU-903						
HFO2	-273.60	HU-006,TR-010	14.17	LA-001	2790.00		S-L	LA-001
HFS2			19.80	TR-003				
HF(CO3)2			34.90	KE-001				
HF(NO2)4								
HF(NO3)4			70.80	RA-004				
HF(SO3)2			45.90	KE-001				
HF(SO4)2			38.80	TR-003				
H2	.00	JA-001	31.21	JA-001				
H2O(GAS)	-57.77	LA-001	45.07	LA-001				
IR	.00		8.50	LA-001	2443.00		S-L	LA-001
IRO2	-53.00	KU-001,TR-010	17.20	LA-001				
IRS2	-34.00	HE-002,TR-010	15.00	HE-002				
IRS3	-26.30	KU-001,LA-001	20.30	LA-001				
IR(SO4)2			39.20	TR-003				
IR2S3	-58.00	HE-002,TR-010	23.00	HE-002,TR-010				
K	.00		15.37	LA-001	63.20 753.80	.56 18.51	S-L L-G	LA-001
KALO2	-271.46	TR-002	18.50	TR-003				
KFEO2	-165.50	TR-002	22.05	TR-003				
KNO2	-88.48	ST-926,LA-908	27.04	RA-003	-13.00 47.00 440.00	1.20 .20	S-S S-S S-L	LA-908,RA-926, PR-903,AD-002
KNO3	-117.70	LA-908	31.76	LA-908	-60.00 127.90 334.30	 1.22 2.30	S-S S-S S-L	LA-908,FE-903, YA-904

COMPOUND	HEAT OF FORMATION 25 DEG.C KCAL/GMOLE	REFERENCES	ABSOLUTE ENTROPY CAL/GMOLE/ DEG. K	REFERENCES	TRANSITION DATA			
					TEMP. DEG.C	HEAT KCAL/ GMOLE	TYPE	REFERENCES
KOH	-101.50	ST-917	18.85	ST-920	249.00	1.51	S-S	ST-917,KU-903
					400.00	2.24	S-L	
					1327.00	32.00	L-G	
KOH[illegible]	-179.50	LA-908			143.00		S-L	LA-908,RO-907
KO[illegible]5H2O	-161.70	RO-907						
K[illegible]H2O	-251.20	RO-907						
[illegible]	-277.33	TR-002	29.90	KE-001				
[illegible]3	-271.87	LA-001	36.07	LA-001	250.00		S-S	LA-001
					428.00		S-S	
					622.00		S-S	
					901.00	7.79	S-L	
K2CRO4	-319.72	TR-002	47.60	KE-001				
K2CR2O4	-541.19	TR-002	44.10	KE-001				
K2MOO4	-356.90	TR-002	43.55	TR-007				
K2O	-86.36	LA-001	23.48	LA-001				
K2S	-87.86	LA-001,TR-010	26.34	TR-003	146.40	.09	S-S	LA-001,KU-001
					835.00		S-L	
K2SO3	-266.90	NB-003	37.40	TR-003				
K2SO4	-342.34	LA-001	41.97	LA-001	595.00	2.25	S-S	LA-001,CA-002
					1069.00	8.75	S-L	
K2TIO3	-384.60	CA-063	32.90	TR-003				
K2WO4	-390.94	TR-002	42.50	TR-007				
LA	.00		13.69	LA-001	548.00		S-S	LA-001
					709.00		S-S	
					920.00	2.70	S-L	
LAN	-71.50	KU-903	11.60	KE-911				
LAS	-108.00	ST-002	18.80	TR-003				
LAS2	-145.00	KU-001,TR-010	18.82	TR-003				
LA(NO2)3	-239.95	RA-002						
LA(NO3)3	-299.83	RA-002	58.80	RA-004				
LA(NO3)3.6H2O					43.00		S-S	RO-907
					66.50		S-L	
LA2O3	-430.50	KU-001,TR-010	30.55	LA-001	2315.00		S-L	LA-001
					4200.00		L-G	

COMPOUND	HEAT OF FORMATION 25 DEG.C KCAL/GMOLE	REFERENCES	ABSOLUTE ENTROPY CAL/GMOLE/ DEG. K	REFERENCES	TRANSITION DATA			
					TEMP. DEG.C	HEAT KCAL/ GMOLE	TYPE	REFERENCES
LA2S3	-282.00	KU-001,TR-010	32.41	TR-003				
LA2(CO3)3			51.60	TR-003				
LA2(SO3)3			60.60	TR-003				
LA2(SO4)3	-939.80	WI-001	68.70	TR-003				
LI	.00		6.70	LA-001	180.50	.72	S-L	LA-001
LIALO2	-284.29	KU-001,LA-001	12.69	LA-001,KU-001				
LIFEO2	-173.70	KU-001	18.00	KU-001				
LINO2	-96.60	ST-926,RO-907	21.34	RA-003	96.00		S-S	ST-926,PR-903
					220.00		S-L	
LINO3	-115.20	LA-908	24.98	RA-003	-10.00		S-S	SC-912,FE-903,
					120.00		S-S	ST-926
					170.00		S-S	
					230.00		S-S	
					253.00	6.04	S-L	
LINO3.3H2O	-328.60	RO-907			29.90	8.33	S-L	NE-904
LIOH	-115.84	ST-917	10.22	ST-917	413.00		S-S	ST-917;LA-908,
					471.30	5.01	S-L	KE-909
					1530.00	40.10	L-G	
LIOH.H2O	-188.90	LA-908	17.07	LA-908,RA-001				
LIVO3	-281.48	TR-002	23.10	KE-001				
LI2CO3	-290.26	LA-001	21.58	LA-001	410.00		S-S	LA-001
					720.00		S-L	
LI2CRO4	-333.53	TR-002	34.00	KE-001				
LI2CR2O4	-501.89	TR-002	30.60	KE-001				
LI2MOO4	-375.52	TR-002	32.15	TR-007				
LI2O	-142.50	LA-001	9.05	LA-001	1727.00	17.99	S-L	LA-001
					2327.00		L-G	
LI2S	-107.40	KU-001	14.94	TR-003				
LI2SO3	-279.40	CA-001	26.00	TR-003				
LI2SO4	-342.58	LA-001	35.36	LA-001	575.00	6.78	S-S	LA-001
					857.00	1.85	S-L	
LI2TIO3	-394.03	TR-002	21.90	LA-001,KU-001				
LI2WO4	-396.56	TR-002	31.10	TR-007				
LI3N	-47.20	ST-918,RO-907	9.00	ST-918,ST-906				

COMPOUND	HEAT OF FORMATION 25 DEG.C KCAL/GMOLE	REFERENCES	ABSOLUTE ENTROPY CAL/GMOLE/ DEG. K	REFERENCES	TRANSITION DATA			
					TEMP. DEG.C	HEAT KCAL/ GMOLE	TYPE	REFERENCES
MG	.00		7.78	LA-001	649.50	2.14	S-L	LA-001
					1120.00	31.49	L-G	
MGAL2O4	-551.00	CA-048,CA-049	19.25	KU-001	2135.00		S-L	KU-001
MGCO3	-263.98	JA-001,LA-001	15.70	JA-001,LA-001				
MGCRO4	-307.08	TR-002	32.00	TR-003				
MGCR2O4	-453.10	CA-038,TR-010	25.30	KU-001,LA-001	2200.00		S-L	KU-001
MGFE2O4	-349.20	CA-042,CA-047	28.28	LA-001	392.00		S-S	LA-001
					957.00	.35	S-S	
MGMOO4	-334.80	CA-077,TR-010	28.40	CA-017				
MGO	-143.63	LA-001,NB-003	6.40	LA-001,NB-003	2802.00	18.49	S-L	LA-001
MGS	-83.00	CA-019,NB-003	10.60	LA-001				
MGSO3	-241.00	NB-003	22.50	TR-003				
MGSO4	-305.50	JA-001	21.90	JA-001	1127.00	3.50	S-L	JA-001
MGTIO3	-371.50	CA-043	17.80	KU-001,LA-001				
MGTI2O5	-600.10	CA-043	30.40	KU-001,LA-001				
MGV2O6	-527.90	CA-050	38.27	CA-051				
MGWO4	-373.40	CA-044	26.86	TR-003				
MG(NO2)2	-153.63	RA-002	37.60	RA-004				
MG(NO3)2	-188.97	SI-926	39.20	LA-908,KE-912				
MG(NO3)2.2H2O	-334.70	MA-928			130.00		S-L	RO-907
MG(NO3)2.6H2O	-624.00	LA-908			90.00	9.80	S-L	LA-908
MG(OH)2	-221.00	ST-918,RA-001	15.10	ST-918				
MG2TIO4			24.80	KU-001				
MG3N2	-110.20	ST-906,LA-908	21.00	ST-906,KU-903	550.00	.11	S-S	KU-903,KE-909
					788.00	.22	S-S	
MN	.00		7.59	LA-001	727.00	.54	S-S	LA-001
					1101.00	.54	S-S	
					1137.00	.43	S-S	
					1244.00	3.49	S-L	
MNAL2O4	-501.10	CA-027	25.18	TR-003	1577.00		S-L	CA-027
MNCO3	-213.74	LA-001	20.47	LA-001				
MNCRO4	-256.88	TR-002	34.75	TR-003				
MNCR2O4	-396.72	TR-002	29.82	TR-003				
MNFE2O4	-293.00	CA-028	31.97	TR-003				

COMPOUND	HEAT OF FORMATION 25 DEG.C KCAL/GMOLE	REFERENCES	ABSOLUTE ENTROPY CAL/GMOLF/ DEG. K	REFERENCES	TRANSITION DATA			
					TEMP. DEG.C	HEAT KCAL/ GMOLE	TYPE	REFERENCES
MNMOO4	-284.40	CA-029	31.27	TR-003				
MNO	-91.93	LA-001	14.26	LA-001	-155.40		S-S	LA-001
					1780.00	13.00	S-L	
MNO2	-124.16	LA-001	12.69	LA-001	250.00		S-S	LA-001
MNS	-49.45	LA-001	18.68	LA-001	1530.00	6.31	S-L	LA-001
MNSO3	-197.37	TR-002	24.40	LR-002				
MNSO4	-253.95	LA-001	26.78	LA-001	460.00	.57	S-S	LA-001,CA-002
					700.00		S-L	
MNS2	-49.50	KU-001	15.32	TR-003				
MNTIO3	-324.30	TR-002	23.20	TR-003				
MNV2O6	-484.18	TR-002	42.38	TR-003				
MNWO4	-312.60	CA-030	29.56	TR-003				
MN(NO2)2	-104.01	RA-002	40.30	RA-004				
MN(NO2)3	-111.56	RA-002						
MN(NO2)4								
MN(NO3)2	-137.73	WA-901,RA-001	45.60	RA-003				
MN(NO3)2.3H2O	-354.90	LA-908			35.50	6.50	S-L	LA-908,RO-907
MN(NO3)2.4H2O					37.10		S-L	RO-907
MN(NO3)2.6H2O	-566.90	WA-901			25.80	9.61	S-L	LA-908,RO-907,
MN(NO3)3	-162.47	RA-002	55.30	RA-004				
MN(NO3)4			66.30	RA-004				
MN(OH)2	-166.20	WA-901	23.70	WA-901,RA-001				
MN(OH)3	-212.00	RO-907						
MN(SO4)2			34.30	TR-003				
MN2O3	-229.11	LA-001	26.40	LA-001	600.00		S-S	LA-001
MN2(AL2O4)3	-1430.00	TR-002	68.40	KE-001				
MN2(CO3)3	-545.46	TR-002	44.60	TR-003				
MN2(CRO4)3	-688.01	TR-002	96.60	KE-001				
MN2(CR2O4)3	-1080.20	TR-002	86.40	KE-001				
MN2(FE2O4)3	-810.67	TR-002	96.60	KE-001				
MN2(MOO4)3	-818.86	TR-002	69.20	TR-007				
MN2(SO3)3	-502.39	TR-002	53.60	TR-003				
MN2(SO4)3	-666.90	WI-001	61.70	TR-003				
MN2(TIO3)3	-906.26	TR-002	60.60	KE-001				

COMPOUND	HEAT OF FORMATION 25 DEG.C KCAL/GMOLE	REFERENCES	ABSOLUTE ENTROPY CAL/GMOLE/ DEG. K	REFERENCES	TRANSITION DATA			
					TEMP. DEG.C	HEAT KCAL/ GMOLE	TYPE	REFERENCES
MN2(V2O6)3	-1369.60	TR-002	133.20	KE-001				
MN2(WO4)3	-862.24	TR-002	66.80	TR-007				
MN3N2								
MN3O4	-331.12	LA-001	35.72	LA-001	1172.00	4.49	S-S	LA-001
					1590.00		S-L	
MN4N	-30.30	MA-925,MA-938	31.00	MA-925				
MN5N2	-48.20	MA-925,RA-001						
MN8N2	-61.50	MA-901,RA-001						
MO	.00		6.83	LA-001	2622.00	6.59	S-L	LA-001
MOO2	-140.85	LA-001	11.06	LA-001				
MOO3	-177.88	LA-001	18.57	LA-001	795.00	12.54	S-L	LA-001
					1155.00	32.97	L-G	
MOS2	-60.40	KU-001,TR-010	16.00	KU-001,LA-001				
MOS3	-61.47	LA-001	15.89	LA-001				
MO(CO3)3			50.10	KE-001				
MO(SO3)3			63.60	TR-003				
MO(SO4)3			67.80	KE-001				
MO2N	-19.50	MA-943,RA-001	21.00	LA-908,KU-903				
MO2S3	-92.50	KU-001,TR-010	28.03	KU-001,LA-001				
NA	.00		12.28	LA-001	97.82	.62	S-L	LA-001
					890.00	21.27	L-G	
NAALO2	-270.67	LA-001,KU-001	16.89	LA-001,KU-001				
NACL	-98.26	JA-001	17.24	JA-001				
NAFEO2	-166.40	TR-002	21.10	LA-001,KU-001				
NANO2	-85.72	ST-926	25.34	RA-003	162.00	.30	S-S	LA-908,RO-907,
					281.00	2.48	S-L	AD-902,ST-926
					-30.00		S-S	SC-912,FE-903
NANO3	-111.85	ST-926	27.80	LA-908,RO-907	160.00		S-S	
					275.00	1.12	S-S	
					306.00	3.69	S-L	
NAOH	-101.90	ST-917	15.40	ST-917,KE-912	292.95	1.52	S-S	ST-917,KU-903,
					319.25	1.52	S-L	LA-908
					1390.00	34.50	L-G	
NAOH.H2O	-175.10	LA-908	20.20	LA-908,RO-907	64.20		S-L	LA-908,RO-907

COMPOUND	HEAT OF FORMATION 25 DEG.C KCAL/GMOLE	REFERENCES	ABSOLUTE ENTROPY CAL/GMOLE/ DEG. K	REFERENCES	TRANSITION DATA			
					TEMP. DEG.C	HEAT KCAL/ GMOLE	TYPE	REFERENCES
NAOH.2H2O			46.86	SI-906	13.50	3.86	S-L	SI-906
NAOH.3H2O			60.99	SI-906	15.50	5.38	S-L	RO-907,SI-906
NAOH.3.5H2O			68.44	SI-906				
NAOH.4H2O			76.17	SI-906				
NAOH.5H2O			92.27	SI-906				
NAOH.7H2O			125.80	SI-906				
NAVO3	-276.47	CA-041	27.40	KE-001				
NA2CO3	-269.72	LA-001,JA-001	32.49	LA-001,JA-001	356.00		S-S	LA-001,JA-001
					486.00		S-S	
					618.00		S-S	
					854.00	7.88	S-L	
NA2CRO4	-318.60	CA-069	42.60	KE-001				
NA2CR2O4	-508.14	TR-002	39.20	KE-001				
NA2MOO4	-354.00	CA-045	38.10	CA-017				
NA2MO2O7	-539.40	CA-045	59.90	CA-046				
NA2O	-102.87	LA-001	16.99	LA-001	920.00	11.20	S-L	LA-001
NA2S	-92.40	KU-001,TR-010	22.48	LA-001	950.00	1.19	S-L	
NA2SO3	-260.40	CA-003,LA-001	34.88	LA-001				
NA2SO4	-330.64	LA-001	35.69	LA-001	259.00	2.64	S-S	LA-001,CA-002
					884.00	6.86	S-L	
NA2TIO3	-379.50	CA-063	29.10	KU-001,LA-001	287.00	.40	S-S	KU-001,LA-001
					1030.00	16.80	S-L	
NA2TI2O5			41.47	KU-001,LA-001	985.00	26.20	S-L	KU-001,LA-001
NA2TI3O7			55.90	KU-001,LA-001	1128.00	37.10	S-L	KU-001
NA2WO4	-382.60	CA-045	39.10	TR-007				
NA2W2O7	-597.30	CA-045	60.80	CA-046				
NB	.00		8.72	LA-001	2487.00	6.40	S-L	LA-001
NBO	-116.11	LA-001	11.99	LA-001				
NBO2	-189.93	LA-001	13.02	LA-001				
NB2O5	-455.10	LA-001	32.78	LA-001	800.00		S-S	LA-001
					1100.00		S-S	
					1512.00	24.58	S-L	
NB2S5			51.80	KE-001				
NB2(CO3)5			85.30	KE-001				

COMPOUND	HEAT OF FORMATION 25 DEG.C KCAL/GMOLE	REFERENCES	ABSOLUTE ENTROPY CAL/GMOLE/ DEG. K	REFERENCES	TRANSITION DATA			
					TEMP. DEG.C	HEAT KCAL/ GMOLE	TYPE	REFERENCES
NO2(SO3)5			107.80	KE-001				
NO2(SO4)5			114.80	KE-001				
NI	.00		7.13	LA-001	357.20	.14	S-S	LA-001
					1455.00	4.25	S-L	
NIAL2O4	-465.32	CA-037	25.38	TR-003				
NICO3	-162.98	LA-001	21.00	LA-001				
NICRO4	-216.48	TR-002	34.95	TR-003				
NICR2O4	-348.74	TR-002	30.02	TR-003				
NIFE2O4	-256.50	CA-036	30.08	LA-001	562.00		S-S	CA-056,LA-001
NIMOO4	-260.26	TR-002	30.77	TR-003				
NIO	-57.26	LA-001	9.08	LA-001	250.00		S-S	LA-001
					1960.00	12.09	S-L	
NIS	-20.20	KU-001,TR-010	12.66	CA-084,TR-010	396.00		S-S	KU-001
NISO3	-155.86	TR-002	25.40	TR-003				
NISO4	-213.50	LA-001	18.59	LA-001				
NITIO3	-287.75	CA-035,CA-055	19.48	CA-035				
NIV2O6	-443.59	TR-002	42.58	TR-003				
NIWO4	-271.62	CA-030	29.76	TR-003				
NI(NO2)2	-61.40	RA-002	40.50	RA-004				
NI(NO3)2	-99.20	WA-901,RA-001	45.80	RA-003				
NI(NO3)2.3H2O	-317.00	WA-901						
NI(NO3)2.6H2O	-528.60	WA-901			56.70		S-L	RO-907
NI(OH)2	-126.60	WA-901	21.00	WA-901				
NI(OH)3	-160.00	WA-901						
NI3N	.20	WA-901,KU-903			440.00		L-G	LA-908
NI3S2	-47.50	KU-001,TR-010	32.00	CA-084,TR-010	550.00		S-S	KU-001
					1984.00		S-L	
NO(G)	21.56	FR-905	50.35	ST-906				
NO2(G)	7.91	ST-906	57.34	ST-906				
N2O3(G)	19.80	ST-906,RA-001	73.91	ST-906	-111.00		S-L	RO-907
					2.00	9.40	L-G	
N2O4(G)	2.17	ST-906	72.72	ST-906				
N2O5	-10.00	RO-907,CO-91	36.60	LA-908	32.40	13.60	S-G	RO-907
N2O5(G)	2.70	ST-906	82.80	ST-906	32.40	13.60	S-G	RO-907

COMPOUND	HEAT OF FORMATION 25 DEG.C KCAL/GMOLE	REFERENCES	ABSOLUTE ENTROPY CAL/GMOLE/ DEG. K	REFERENCES	TRANSITION DATA			
					TEMP. DEG.C	HEAT KCAL/ GMOLE	TYPE	REFERENCES
N2(GAS)	.00	JA-001	45.77	JA-001				
O2	.00		48.97	LA-001				
PB	.00		15.51	LA-001	327.40	1.14	S-L	LA-001
					1751.00	42.88	L-G	
PBAL2O4	-459.57	TR-002	30.38	TR-003				
PBCO3	-167.23	LA-001,NB-002	31.27	LA-001,NB-002				
PBCO3*PBO	-219.84	LA-001	48.47	LA-001				
PBCO3*2PBO	-272.82	LA-001	64.98	LA-001				
PBCRO4	-217.50	LA-001	39.95	TR-003	707.00		S-S	LA-001
PBCR2O4	-357.23	TR-002	35.02	TR-003				
PBFE2O4	-251.22	TR-002	37.17	TR-003				
PBMOO4	-265.65	LA-001	35.77	TR-003	1065.00		S-L	LA-001
PBO	-52.37	LA-001	15.60	LA-001	489.00		S-S	LA-001
					890.00	2.80	S-L	
					1472.00	50.89	L-G	
PBO*PBSO4	-275.20	KE-003	51.97	KE-003	970.00		S-L	LA-001
PBO2	-66.08	LA-001	18.26	LA-001				
PBS	-22.52	LA-001,NB-003	21.79	NB-003,LA-001	1114.00	4.16	S-L	LA-001,NB-003
PBSO3	-157.00	CA-006	30.40	TR-003				
PBSO4	-219.33	LA-001	35.17	LA-001	881.00	7.30	S-S	LA-001,CA-002
					1087.00	9.60	S-L	
PBTIO3	-285.34	TR-002	28.41	TR-003	490.00	1.15	S-S	LA-001,KU-001
					1170.00		S-L	
PBV2O6	-445.55	TR-002	47.58	TR-003				
PBWO4	-277.49	TR-002	34.76	TR-003				
PB(NO2)2	-66.10	RA-002	45.50	RA-004				
PB(NO2)4								
PB(NO3)2	-108.00	ST-926,WA-918	50.80	RA-003				
PB(NO3)4			71.50	RA-004				
PB(OH)2	-123.30	WA-918	21.00	LA-908,RO-907				
PB(SO4)2			59.50	TR-003				
PB3O4	-175.47	LA-001	50.46	LA-001				
PD	.00		9.03	LA-001	1555.00	4.11	S-L	LA-001
PDCO3			24.09	TR-003				

COMPOUND	HEAT OF FORMATION 25 DEG.C KCAL/GMOLE	REFERENCES	ABSOLUTE ENTROPY CAL/GMOLE/ DEG. K	REFERENCES	TRANSITION DATA			
					TEMP. DEG.C	HEAT KCAL/ GMOLE	TYPE	REFERENCES
PDO	-27.60	HE-002,TR-010	13.37	LA-001				
PDS	-18.00	HE-002	17.72	TR-003				
PDSO3			27.60	TR-003				
PDSO4			28.70	TR-003				
PDS2	-19.00	HE-002	17.72	TR-003				
RBNO2	-86.71	ST-926	29.74	HA-003	422.00		S-L	PH-903
RBNO3	-117.00	LA-908	33.38	HA-003	160.00	.93	S-S	ST-92.
					215.00	.77	S-S	
					281.00	.23	S-S	
					310.00	1.11	S-L	
RBOH	-98.87	LA-908,RO-907			245.00	1.70	S-S	LA-908,RO-907
					301.00	1.62	S-L	
RBOH,H2O	-177.80	RO-907						
RBOH,2H2O	-250.80	RO-907						
RB2CO3	-269.48	LA-001	39.83	TR-003	303.00		S-S	LA-001
					873.00		S-L	
RB2O	-78.84	LA-001	26.50	TR-003	567.00	8.50	S-L	LA-001
RB2S	-83.20	NB-003,KU-001	31.70	TR-003				
RB2SO3	-265.32	TR-002	42.80	TR-003				
RB2SO4	-340.50	RO-907,LA-908	47.53	TR-003	650.00		S-S	LA-001,CA-002
					881.00	2.11	S-S	
					1074.00		S-L	
RE	.00		8.88	LA-001	3180.00	9.08	S-L	LA-001
REO2	-101.46	LA-001	17.39	LA-001				
REO3	-145.94	LA-001	19.30	LA-001	160.00		S-L	LA-001
RES2	-42.70	CA-074,TR-010	19.22	LA-001				
RES3	-49.80	KU-001	23.00	KU-001				
RE2O7	-295.76	LA-001	49.52	LA-001	300.30	15.80	S-L	LA-001
					360.30	17.70	L-G	
RE2O8	-148.24	LA-001			150.00		S-L	LA-001
RE2S7	-107.90	CA-074,KU-001	48.00	KU-001				
RH	.00		7.55	LA-001	1960.00		S-L	LA-001
RHCO3			23.89	TR-003				
RHO	-23.89	LA-001	12.90	LA-001				

COMPOUND	HEAT OF FORMATION 25 DEG.C KCAL/GMOLE	REFERENCES	ABSOLUTE ENTROPY CAL/GMOLE/ DEG. K	REFERENCES	TRANSITION DATA			
					TEMP. DEG.C	HEAT KCAL/ GMOLE	TYPE	REFERENCES
RHS			17.52	TR-003				
RHSO3			27.40	TR-003				
RHSO4			28.50	TR-003				
RH2O	-22.67	LA-001	27.70	TR-003				
RH2O3	-70.95	LA-001	26.50	TR-003				
RH2S			32.94	TR-003				
RH2SO4			48.69	TR-003				
RH2S3			29.80	TR-003				
RH2(SO4)3			66.10	TR-003				
RU	.00		6.82	LA-001	1035.00	.03	S-S	LA-001
					1200.00		S-S	
					1500.00	.23	S-S	
					2500.00		S-L	
RUO2	-72.20	CA-082,CA-083	12.50	CA-016				
RUO3(GAS)	-18.00	CA-016	63.70	CA-016				
RUO4(GAS)	-46.70	CA-016	65.50	CA-016,OR-001				
RUS2	-40.00	KU-001,TR-010	10.40	HE-002,TR-010				
S	.00	NB-003,JA-001	7.63	LA-001,NB-003	95.31	.10	S-S	LA-001
					101.00	.00	S-S	
					115.18	.41	S-L	
					444.60		L-G	
SB	.00		10.92	LA-001	94.60		S-S	LA-001
					413.00		S-S	
					630.90	4.88	S-L	
SB2O3	-169.40	CA-060	31.65	CA-010				
SB2O4	-216.90	CA-060,TR-010	30.20	LA-001				
SB2O5	-210.23	LA-001	29.89	LA-001				
SB2S3	-40.50	KU-001,TR-010	43.50	CA-073,TR-010	546.00	5.60	S-L	LA-001,KU-001
SB2(AL2O4)3	-1362.50	TR-002	71.40	KE-001				
SB2(CO3)3	-468.09	TR-002	50.40	TR-003				
SB2(CRO4)3	-611.09	TR-002	99.60	KE-001				
SB2(CR2O4)3	-997.12	TR-002	89.40	KE-001				
SB2(FE2O4)3	-737.07	TR-002	99.60	KE-001				
SB2(MOO4)3	-740.01	TR-002	75.00	TR-007				

DATE 6 OCT. 1971 HEAT OF FORMATION, ENTROPY, AND TRANSITION DATA (CONTINUED) PAGE: 23

COMPOUND	HEAT OF FORMATION 25 DEG.C KCAL/GMOLE	REFERENCES	ABSOLUTE ENTROPY CAL/GMOLE/ DEG. K	REFERENCES	TRANSITION DATA			
					TEMP. DEG.C	HEAT KCAL/ GMOLE	TYPE	REFERENCES
SB2(SO3)3	-420.64	TR-002	59.40	TR-003				
SB2(SO4)3	-574.20	NB-001,WI-001	67.50	TR-003				
SB2(TIO3)3	-839.04	TR-002	63.60	KE-001				
SB2(V2O6)3	-1294.40	TR-002	136.20	KE-001				
SB2(WO4)3	-785.00	TR-002	72.60	TR-007				
SC	.00	KR-001	8.20	KE-004,LA-001				
SC2O3	-456.16	HU-004,TR-010	18.40	CA-014				
SC2(CO3)3			43.40	TR-003				
SC2(SO3)3			52.40	TR-003				
SC2(SO4)3			60.50	TR-003				
SI	.00		4.47	LA-001	1423.00	11.11	S-L	LA-001
SIO(GAS)	-23.20	KU-001,LA-001	50.55	KU-001				
SIO2	-217.72	KU-001,TR-010	10.00	LA-001,NB-002	867.00	.12	S-S	LA-001
					1610.00	2.04	S-L	
SIS(GAS)	16.93	JA-001	53.43	JA-001				
SIS2	-49.00	JA-001,KU-001	18.00	KE-001,TR-003	1090.00		S-L	
SI(CO3)2			31.20	KE-001				
SI(SO3)2			40.20	KE-001				
SI(SO4)2			32.10	TR-003				
SN	.00		12.20	LA-001	18.00	.60	S-S	LA-001
					202.00	.00	S-S	
					231.90	1.69	S-L	
SNCO3			24.49	TR-003				
SNO	-68.35	LA-001,NB-002	13.56	LA-001,NB-002	1465.00	38.46	L-G	LA-001
SNO2	-138.75	LA-001,NB-001	12.50	LA-001,NB-001	410.00	.45	S-S	LA-001
SNS	-24.32	LA-001,WI-001	18.40	LA-001,KU-001	584.00	.16	S-S	LA-001,KU-001
					880.00	7.55	S-L	
SNSO3			28.00	TR-003				
SNSO4			29.10	TR-003				
SNS2	-39.90	LA-001,KU-001	20.88	LA-001,KU-001				
SN(AL2O4)2	-926.28	TR-002	40.90	KE-001				
SN(CO3)2	-330.04	TR-002	33.90	KE-001				
SN(CRO4)2	-425.63	TR-002	59.70	KE-001				
SN(CR2O4)2	-684.03	TR-002	52.90	KE-001				

DATE 6 OCT. 1971 HEAT OF FORMATION, ENTROPY, AND TRANSITION DATA (CONTINUED) PAGE: 24

COMPOUND	HEAT OF FORMATION 25 DEG.C KCAL/GMOLE	REFERENCES	ABSOLUTE ENTROPY CAL/GMOLE/ DEG. K	REFERENCES	TRANSITION DATA			
					TEMP. DEG.C	HEAT KCAL/ GMOLE	TYPE	REFERENCES
SN(FE2O4)2	-507.28	TR-002	59.70	KE-001				
SN(MOO4)2	-509.39	TR-002	39.00	TR-007				
SN(NO2)2			43.10	RA-004				
SN(NO2)4	-109.98	RA-002						
SN(NO3)2			48.40	RA-003				
SN(NO3)4	-167.26	RA-002	69.10	RA-004				
SN(OH)2	-134.10	WA-918	57.00	WA-918	91.00		S-L	ST-926
SN(OH)4	-265.30	WA-918						
SN(SO3)2	-295.36	TR-002	42.90	KE-001				
SN(SO4)2	-393.40	NB-004,WI-001	37.10	TR-003				
SN(TIO3)2	-577.14	TR-002	35.70	KE-001				
SN(V2O6)2	-884.00	TR-002	84.10	KE-001				
SN(WO4)2	-542.46	TR-002	37.70	TR-007				
SO2	-70.93	LA-001	59.27	LA-001				
SO3	-94.41	LA-001	61.16	LA-001				
SR	.00		13.00	LA-001	589.00	.20	S-S	LA-001
					770.00	2.20	S-L	
					1367.00	33.18	L-G	
SRAL2O4	-559.81	CA-022	26.88	TR-003				
SRCO3	-290.98	LA-001	23.17	LA-001	924.00	.40	S-S	LA-001
					1497.00		S-L	
SRCRO4	-333.36	TR-002	36.45	TR-003				
SRCR2O4	-514.63	TR-002	31.52	TR-003				
SRFE2O4	-356.06	TR-002	33.67	TR-003				
SRMOO3	-308.60	CA-024						
SRMOO4	-375.20	TR-002	32.27	TR-003				
SRO	-140.74	LA-001,CA-007	13.00	LA-001	2460.00	16.70	S-L	LA-001
					3200.00	126.62	L-G	
SRS	-108.10	KU-001,TR-010	16.50	KU-001,LA-001				
SRSO3	-279.40	CA-006	26.90	TR-003				
SRSO4	-344.97	LA-001	29.07	LA-001	1152.00		S-S	LA-001,CA-002
					1605.00		S-L	
SRTIO3	-393.50	TR-002	25.99	LA-001				
SRV2O6	-562.96	TR-002	44.08	TR-003				

COMPOUND	HEAT OF FORMATION 25 DEG.C KCAL/GMOLE	REFERENCES	ABSOLUTE ENTROPY CAL/GMOLE/ DEG. K	REFERENCES	TRANSITION DATA TEMP. DEG.C	HEAT KCAL/ GMOLE	TYPE	REFERENCES
SRWO4	-393.00	CA-023	28.30	CA-023				
SR(NO2)2	-182.20	ST-926	42.00	RA-004	274.00		S-S	ST-926
					288.00		S-S	
					403.00		S-L	
SR(NO3)2	-233.80	ST-926	46.50	TA-913	645.00	10.65	S-L	ST-926,RO-907,
SR(NO3)2,4H20	-519.50	RO-907						
SR(OH)2	-229.30	RO-907			535.00	5.49	S-L	KE-909
SR(OH)2.H20	-502.30	RO-907						
SR(OH)2.8H20	-801.20	RO-907						
SR2TIO4			38.00	KU-001,LA-001				
SR3N2	-93.40	KU-903,RA-001			1030.00		S-L	KU-903
S(GAS)	52.80	LA-001	40.09	LA-001				
TA	.00		9.89	LA-001	2996.00	7.50	S-L	LA-001
TAN	-59.00	KU-903,RA-001	12.20	KU-903	3090.00		S-L	LA-908,KU-903
TA2N	-64.70	KU-903,MA-943						
TA2O5	-488.50	KU-001,TR-010	34.15	LA-001	1320.00		S-S	LA-001
					1880.00		S-L	
TA2S5			53.20	KE-001				
TA2(CO3)5			86.70	KE-001				
TA2(SO3)5			109.20	KE-001				
TA2(SO4)5			116.20	KE-001				
TH	.00		12.75	LA-001	225.00		S-S	LA-001
					1400.00	.67	S-S	
					1695.00	3.74	S-L	
THO2	-294.09	LA-001	15.59	LA-001	2950.00		S-L	LA-001
					4400.00		L-G	
THS	-99.96	LA-001	20.92	TR-003				
THS2	-109.89	LA-001	20.92	TR-003	1905.00		S-L	LA-001,KU-001
TH(AL2O4)2	-1101.50	TR-002	44.50	KE-001				
TH(CO3)2	-519.62	TR-002	37.50	KE-001				
TH(CRO4)2	-614.33	TR-002	63.30	KE-001				
TH(CR2O4)2	-884.49	TR-002	56.50	KE-001				
TH(FE2O4)2	-687.28	TR-002	63.30	KE-001				
TH(MOO4)2	-701.89	TR-002	41.80	TR-007				

COMPOUND	HEAT OF FORMATION 25 DEG.C KCAL/GMOLE	REFERENCES	ABSOLUTE ENTROPY CAL/GMOLE/ DEG. K	REFERENCES	TRANSITION DATA TEMP. DEG.C	HEAT KCAL/ GMOLE	TYPE	REFERENCES
TH(SO3)2	-495.41	TR-002	46.50	KE-001				
TH(SO4)2	-607.26	CA-011	35.40	CA-011				
TH(TIO3)2	-752.68	TR-002	39.30	KE-001				
TH(V2O6)2	-1068.60	TR-002	87.70	KE-001				
TH(WO4)2	-731.63	TR-002	40.50	TR-007				
TH2S3	-258.60	LA-001,NB-003	36.60	TR-003	1950.00		S-L	LA-001,KU-001
TI	.00		7.32	LA-001	882.00	.95	S-S	JA-001,LA-001
					1668.00	3.70	S-L	
TICO3			21.19	TR-003				
TIN	-80.70	ST-919,RA-001	7.23	ST-919	2947.00	16.00	S-L	ST-919
TIO	-123.85	LA-001	8.30	LA-001	991.00	.82	S-S	LA-001
					2020.00	13.98	S-L	
TIO2	-225.50	LA-001	12.00	LA-001	1855.00	15.48	S-L	LA-001
TISO3			24.70	TR-003				
TISO4			25.80	TR-003				
TIS2	-80.00	KU-001	18.73	LA-001,KU-001	147.00		S-S	KU-001
TI(NO2)2			39.80	RA-004				
TI(NO2)3								
TI(NO2)4								
TI(NO3)2			45.10	RA-003				
TI(NO3)3			54.80	RA-004				
TI(NO3)4			65.80	RA-004	58.00		S-L	ST-926
TI(SO4)2			33.80	TR-003				
TI2O3	-362.65	LA-001,JA-001	18.82	LA-001,JA-001	200.00	.22	S-S	LA-001,JA-001
					2130.00	38.46	S-L	
TI2(CO3)3			43.60	TR-003				
TI2(SO3)3			52.60	TR-003				
TI2(SO4)3			60.70	TR-003				
TI3O5	-586.74	LA-001	30.89	LA-001	177.00	.22	S-S	LA-001
U	.00		12.02	LA-001	662.00	.70	S-S	LA-001
					772.00	1.14	S-S	
					1133.00	4.71	S-L	
UO2	-258.97	LA-001	18.62	LA-001	2730.00		S-L	LA-001
UO2SO4	-451.20	OW-001	36.57	OW-001				

COMPOUND	HEAT OF FORMATION 25 DEG.C KCAL/GMOLE	REFERENCES	ABSOLUTE ENTROPY CAL/GMOLE/DEG. K	REFERENCES	TRANSITION DATA			
					TEMP. DEG.C	HEAT KCAL/GMOLE	TYPE	REFERENCES
UO3	-291.70	LA-001	23.55	LA-001				
US	-91.00	CA-075,KU-001	18.00	KU-001	2462.00		S-L	CA-075
US2	-120.00	KU-001	26.00	KU-001	1350.00		S-S	KU-001
					1680.00		S-L	
U(AL2O4)2	-1063.00	TR-002	48.00	KE-001				
U(CO3)2	-478.20	TR-002	51.00	KE-001				
U(CRO4)2	-573.04	TR-002	66.80	KE-001				
U(CR2O4)2	-839.00	TR-002	60.00	KE-001				
U(FE2O4)2	-650.72	TR-002	66.80	KE-001				
U(MOO4)2	-660.57	TR-002	41.90	TR-007				
U(SO3)2	-461.00	TR-002	50.00	KE-001				
U(SO4)2	-563.00	WI-001	40.00	TR-003				
U(TIO3)2	-714.04	TR-002	42.80	KE-001				
U(V2O6)2	-1027.20	TR-002	91.20	KE-001				
U(WO4)2	-689.78	TR-002	40.60	TR-007				
U2S3	-224.00	KU-001	35.00	KU-001				
U3O8	-854.10	KU-001	67.50	KU-001,LA-001				
V	.00		7.00	LA-001	1730.00	4.18	S-L	LA-001
VCO3			21.49	TR-003				
VN			8.91	KU-903,KE-912	2050.00		S-L	LA-908,KU-903
VO	-97.95	LA-001	9.29	LA-001	3100.00		L-G	LA-001
VOSO4	-313.10	FL-001	27.10	FL-001				
VS	-44.91	LA-001	14.50	LA-001	1900.00		S-L	LA-001
VSO3			25.00	TR-003				
VSO4			26.10	TR-003				
V2O3	-289.79	LA-001	23.48	LA-001	1967.00		S-L	LA-001
V2O4	-343.78	LA-001	24.50	LA-001	72.00	2.05	S-S	LA-001
					1542.00	27.19	S-L	
					2700.00		L-G	
V2O5	-372.68	LA-001,NB-003	31.27	LA-001,NB-003	670.00	15.55	S-L	LA-001
					1800.00		L-G	
V2S3			25.00	TR-003				
V2S4			30.20	TR-003				
V2S5			50.20	KE-001				

COMPOUND	HEAT OF FORMATION 25 DEG.C KCAL/GMOLE	REFERENCES	ABSOLUTE ENTROPY CAL/GMOLE/DEG. K	REFERENCES	TRANSITION DATA			
					TEMP. DEG.C	HEAT KCAL/GMOLE	TYPE	REFERENCES
V2(CO3)3			44.10	TR-003				
V2(SO3)3			53.20	TR-003				
V2(SO4)3			61.30	TR-003				
W	.00		7.85	LA-001	3377.00	8.42	S-L	JA-001
WO2	-140.90	KU-001,TR-010	16.01	LA-001				
WO3	-201.46	JA-001	18.14	JA-001	777.00	.41	S-S	JA-001
					1472.00	17.55	S-L	
					1667.00	20.70	L-G	
WS2	-53.97	CA-070,TR-010	28.90	CA-070,TR-010				
W(CO3)2			33.10	KE-001				
W(CO3)3			49.70	KE-001				
W(SO3)2			42.10	KE-001				
W(SO3)3			63.20	KE-001				
W(SO4)2			39.00	TR-003				
W(SO4)3			67.40	KE-001				
Y	.00	LA-001	10.99	LA-001				
Y2O3	-455.34	LA-001,KU-001	23.68	LA-001,KU-001				
Y2(CO3)3			48.00	TR-003				
Y2(SO3)3			57.00	TR-003				
Y2(SO4)3			65.10	TR-003				
ZN	.00		9.94	LA-001	419.50	1.74	S-L	LA-001
					907.00	27.40	L-G	
ZNAL2O4	-485.00	TR-002	25.78	TR-003				
ZNCO3	-193.68	LA-001,NB-003	19.69	LA-001,NB-003				
ZNCRO4	-239.65	TR-002	35.35	TR-003				
ZNCR2O4	-372.83	TR-002	30.42	TR-003				
ZNFE2O4	-279.60	CA-028,TR-010	32.20	KU-001,LA-001				
ZNMOO4	-283.39	TR-002	31.17	TR-003				
ZNO	-83.38	LA-001	10.39	LA-001	1975.00	12.49	S-L	LA-001
ZNO*2ZNSO4	-551.36	IN-002	66.44	IN-002				
ZNS	-48.50	LA-001,NB-003	13.80	LA-001,NB-003				
ZNSO3	-178.48	TR-002	25.80	TR-003				
ZNSO4	-233.69	LA-001,NB-003	29.77	LA-001,NB-003	754.00	4.74	S-S	CA-002
ZNTIO3	-309.30	CA-039	24.21	TR-003				

COMPOUND	HEAT OF FORMATION 25 DEG.C KCAL/GMOLE	REFERENCES	ABSOLUTE ENTROPY CAL/GMOLE/ DEG. K	REFERENCES	TRANSITION DATA TEMP. DEG.C	HEAT KCAL/ GMOLE	TYPE	REFERENCES
ZNV2O6	-466.75	TR-002	42.98	TR-003				
ZNWO4	-327.00	CA-040	33.80	CA-040				
ZN(NO2)2	-83.58	RA-002	40.90	RA-004				
ZN(NO3)2	-115.60	ST-926,WA-918	46.20	RA-003				
ZN(NO3)2.H2O	-192.40	WA-918			70.70		S-L	LA-908,RO-907
ZN(NO3)2.2H2O	-265.36	WA-918			55.40		S-L	RO-907
ZN(NO3)2.4H2O	-406.10	WA-918			44.70		S-L	RO-907
ZN(NO3)2.6H2O	-551.30	WA-918	109.20	WA-918	36.10		S-L	RO-907
ZN(OH)2	-153.74	WA-918	19.50	WA-918				
ZN2TIO4	-391.90	CA-039	32.78	LA-001,KU-001				
ZN3N2	-5.40	WA-918,HA-001						
ZR	.00	LA-001	9.29	LA-001	862.00	.91	S-S	LA-001
					1855.00	4.78	S-L	
ZRN	-87.30	ST-906,KU-903	9.29	ST-906,KE-912	2952.00	16.10	S-L	ST-906
ZRO2	-261.36	LA-001	12.02	LA-001				
ZRS2			17.12	TR-003				
ZR(AL2O4)2	-1078.30	TR-002	39.50	KE-001				
ZR(CO3)2	-502.61	TR-002	32.50	KE-001				
ZR(CRO4)2	-596.97	TR-002	58.30	KE-001				
ZR(CR2O4)2	-879.29	TR-002	51.50	KE-001				
ZR(FE2O4)2	-661.04	TR-002	58.30	KE-001				
ZR(MOO4)2	-684.18	TR-002	38.00	TR-007				
ZR(NO2)2			42.10	RA-004				
ZR(NO2)4	-291.16	RA-002						
ZR(NO3)2			47.40	RA-003				
ZR(NO3)2.6H2O					36.40		S-L	RO-907
ZR(NO3)4	-370.06	RA-002	68.10	RA-004				
ZR(OH)4	-411.20	RO-907						
ZR(OH)4.H2O	-482.90	RO-907						
ZR(OH)4.2H2O	-554.20	RO-907						
ZR(SO3)2	-478.52	TR-002	41.50	KE-001				
ZR(SO4)2	-597.01	LA-001	36.10	TR-003				
ZR(TIO3)2	-729.98	TR-002	34.30	KE-001				
ZR(V2O6)2	-1051.90	TR-002	82.70	KE-001				

COMPOUND	HEAT OF FORMATION 25 DEG.C KCAL/GMOLE	REFERENCES	ABSOLUTE ENTROPY CAL/GMOLE/ DEG. K	REFERENCES	TRANSITION DATA TEMP. DEG.C	HEAT KCAL/ GMOLE	TYPE	REFERENCES
ZR(WO4)2	-716.02	TR-002	36.70	TR-007				
ZR3N2								

TABLE VI

HEAT CAPACITY (CAL/GMOLE/DEG.K)

EQUATION CP = A + BT + CT**2 - D/T**2

COMPOUND	A	COEFFICIENTS BX10**3	CX10**6	DX10**-5	TEMPERATURE RANGE DEGREES CENTIGRADE			REFERENCES
AG	5.38	1.74	.00	-.17	25.00	TO	961.28	LA-001,PE-001
	7.50	.00	.00	.00	961.28	TO	1200.00	
AGNO2	3.65	28.70	.00	-2.47	59.00	TO	200.00	RA-005
AGNO3	8.76	45.18	.00	.00	25.00	TO	210.00	LA-908
	30.58	.00	.00	.00	210.00	TO	327.00	
AGVO3	31.11	3.88	.00	7.45	25.00	TO	700.00	TR-004
AG2AL2O4	39.66	11.38	.00	7.92	25.00	TO	700.00	TR-004
AG2CO3	19.57	24.36	.00	.00	25.00	TO	227.00	LA-001,KU-002
AG2CRO4	34.54	12.44	.00	4.96	25.00	TO	700.00	TR-004
AG2CR2O4	41.78	9.24	.00	3.74	25.00	TO	700.00	TR-004
AG2FE2O4	39.71	21.79	.00	5.60	25.00	TO	700.00	TR-004
AG2MOO4	33.51	12.94	.00	3.68	25.00	TO	700.00	TR-004
AG2O	13.25	7.04	.00	.00	25.00	TO	700.00	LA-001
AG2S	10.13	26.40	.00	.00	25.00	TO	179.00	KU-001,LA-001
	21.64	.00	.00	.00	179.00	TO	577.00	
AG2SO3	20.16	22.14	.00	.00	25.00	TO	[illegible]	TR-001
AG2SO4	23.39	27.58	.00	.24	25.00	TO	657.00	LA-001
AG2TIO3	30.39	8.02	.00	3.50	25.00	TO	700.00	TR-004
AG2WO4	35.55	8.97	.00	4.80	25.00	TO	700.00	TR-004
AL	4.95	2.95	.00	.01	25.00	TO	658.60	LA-001,PE-001
	7.00	.00	.00	.00	658.60	TO	727.00	
ALN	6.66	3.62	.00	.57	.00	TO	1727.00	ST-906
AL(NO2)3	4.27	77.70	.00	-3.85	59.00	TO	200.00	RA-005
AL(NO3)3	63.09	27.57	.00	20.55	25.00	TO	627.00	RA-005
AL(NO3)3.6H2O	16.29	290.80	.00	.11	.00	TO	24.99	LA-908
AL(NO3)3.9H2O						TO		
AL(OH)3						TO		
AL2O3	26.40	4.34	.00	7.92	25.00	TO	700.00	LA-001,NB-002
AL2S						TO		

EQUATION CP = A + BT + CT**2 - D/T**2

COMPOUND	A	COEFFICIENTS BX10**3	CX10**6	DX10**-5	TEMPERATURE RANGE DEGREES CENTIGRADE			REFERENCES
AL2S3	31.99	.98	.00	7.28	25.00	TO	700.00	TR-009
AL2TIO5	43.54	5.28	.00	11.42	25.00	TO	700.00	TR-004
AL2(CO3)3	65.57	21.94	.00	25.23	25.00	TO	700.00	TR-001
AL2(CRO4)3	90.26	20.54	.00	22.79	25.00	TO	700.00	TR-004
AL2(CR2O4)3	111.98	10.93	.00	19.14	25.00	TO	700.00	TR-004
AL2(FE2O4)3	105.78	48.60	.00	24.74	25.00	TO	700.00	TR-004
AL2(MOO4)3	86.59	22.03	.00	18.96	25.00	TO	700.00	TR-004
AL2(SO3)3	47.14	49.64	.00	7.92	25.00	TO	700.00	TR-001
AL2(SO4)3	87.51	14.96	.00	26.66	25.00	TO	700.00	LA-001
AL2(TIO3)3	77.80	7.28	.00	18.41	25.00	TO	700.00	TR-004
AL2(V2O6)3	173.32	6.52	.00	52.64	25.00	TO	700.00	TR-004
AL2(WO4)3	93.30	10.13	.00	22.31	25.00	TO	700.00	TR-004
AS	5.23	2.22	.00	.01	25.00	TO	500.00	LA-001,PE-001
AS2O3	8.37	48.60	.00	.00	25.00	TO	300.00	KU-001
AS2O5						TO		
AS2S3	13.95	45.20	.00	-.64	25.00	TO	300.00	TR-009
AS2S5						TO		
AS2(CO3)3	47.54	66.20	.00	17.31	25.00	TO	300.00	TR-001
AS2(SO3)3	29.10	93.90	.00	.00	25.00	TO	300.00	TR-001
AS2(SO4)3	36.27	101.86	.00	1.74	25.00	TO	300.00	TR-001
B	1.46	4.52	.00	-.04	25.00	TO	700.00	LA-001,PE-001
BA	5.43	3.15	.00	.07	25.00	TO	370.00	LA-001
	2.46	6.98	.00	-.17	370.00	TO	710.00	
	7.50	.00	.00	.00	710.00	TO	1200.00	
BAAL2O4	39.14	5.38	.00	9.91	25.00	TO	700.00	TR-004
BACO3	20.76	11.69	.00	4.77	25.00	TO	700.00	LA-001
BACRO4	34.02	6.44	.00	6.94	25.00	TO	700.00	TR-004
BACR2O4	41.26	3.24	.00	5.72	25.00	TO	700.00	TR-004
BAFE2O4	39.19	15.79	.00	7.59	25.00	TO	700.00	TR-004
BAMOO3						TO		

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DATE  6  OCT.  1971        HEAT CAPACITY (CAL/GMOLE/DEG.K) CONTINUED                        PAGE:    3

                           EQUATION  CP =  A  +  BT  +  CT**2  -  D/T**2

   COMPOUND                      COEFFICIENTS                          TEMPERATURE  RANGE      REFERENCES
                      A          BX10**3     CX10**6   DX10**-5       DEGREES CENTIGRADE

BACRO4              32.79         6.94        .00        5.66       25.00    TO     700.00  TR-004
BAO                 12.73         1.04        .00        1.98       25.00    TO     700.00  LA-001

BAS                 14.59         -.08        .00        1.77       25.00    TO     700.00  TR-009
BASO3               19.64        10.14        .00        1.98       25.00    TO     700.00  TR-001
BASO4               33.76          .03        .00        8.39       25.00    TO     700.00  LA-001
BATIO3              29.03         2.04        .00        4.58       25.00    TO    1500.00  KU-001
BAV2O6              61.70         1.76        .00       16.09       25.00    TO     700.00  TR-004

BAWO4               35.02         2.97        .00        6.80       25.00    TO     700.00  TR-004
BA(NO2)2             6.78        51.40        .00       -2.96       59.00    TO     200.00  RA-005
BA(NO2)2.H2O                                                                 TO
BA(NO3)2            30.05        35.70        .00        4.01       25.00    TO     577.00  KE-909
BA(OH)2             16.90        21.90        .00         .00       25.00    TO     417.00  KE-909
                    32.30          .00        .00         .00      417.00    TO     927.00

BA(OH)2.H2O                                                                  TO
BA(OH)2.8H2O                                                                 TO
BA2TIO4             42.60         3.06        .00        7.96       25.00    TO     700.00  TR-004
BA3N2
BE                   4.61         2.09        .00        1.13       25.00    TO    1200.00  LA-001,PE-001

BEAL2O4             34.65         8.34        .00       11.09       25.00    TO     700.00  TR-004
BECO3               21.50         4.67        .00        8.94       25.00    TO     700.00  TR-001
BECRO4              29.73         9.40        .00        8.12       25.00    TO     700.00  TR-004
BECR2O4             36.97         6.20        .00        6.91       25.00    TO     700.00  TR-004
BEFE2O4             34.90        18.75        .00        8.77       25.00    TO     700.00  TR-004

BEMOO4              28.51         9.30        .00        6.35       25.00    TO     700.00  TR-004
BEO                  8.45         4.00        .00        3.17       25.00    TO     700.00  LA-001,CA-012
BES                 10.31         2.65        .00        2.35       25.00    TO     700.00  TR-009
BESO3               15.36        19.10        .00        3.17       25.00    TO     700.00  TR-001
BESO4               14.47        28.32        .00        2.15       25.00    TO     600.00  CA-005

BETIO3              25.58         4.96        .00        6.67       25.00    TO     700.00  TR-004
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DATE  6  OCT.  1971        HEAT CAPACITY (CAL/GMOLE/DEG.K) CONTINUED                        PAGE:    4

                           EQUATION  CP =  A  +  BT  +  CT**2  -  D/T**2

   COMPOUND                      COEFFICIENTS                          TEMPERATURE  RANGE      REFERENCES
                      A          BX10**3     CX10**6   DX10**-5       DEGREES CENTIGRADE

BEV2O6              57.42         4.72        .00       18.07       25.00    TO     700.00  TR-004
BEWO4               30.74         5.05        .00        7.96       25.00    TO     700.00  TR-004
BE(NO2)2             2.49        54.36        .00       -1.77       59.00    TO     200.00  RA-005
BE(NO3)2            41.70        20.93        .00       14.23       25.00    TO     627.00  RA-005

BE(OH)2              2.29        53.57        .00       -3.00       24.84    TO     134.00  ST-918
                    15.30        16.05        .00        4.23      134.00    TO     526.80
BE3N2               15.00        10.64        .00        1.54         .00    TO    1727.00  ST-918,ST-906
BI                   4.48         5.40        .00        -.00       25.00    TO     271.30  LA-001,PE-001
                     7.50          .00        .00         .00      271.30    TO     700.00
BI(NO2)3             3.43        79.50        .00       -7.00       59.00    TO     200.00  RA-005
BI(NO3)3            62.25        29.40        .00       16.59       25.00    TO     500.00  RA-005

BI(OH)3                                                                      TO
BI2O3               24.73         8.00        .00         .00       25.00    TO     500.00  LA-001
BI2S3               28.89         6.10        .00         .01       25.00    TO     600.00  KU-001,LA-001
BI2(AL2O4)3        103.94        21.02        .00       23.77       25.00    TO     500.00  TR-004
BI2(CO3)3           63.89        25.59        .00       17.31       25.00    TO     500.00  TR-001

BI2(CRO4)3          88.58        24.19        .00       14.37       25.00    TO     700.00  TR-004
BI2(CR2O4)3        110.30        14.53        .00       11.22       25.00    TO     500.00  TR-004
BI2(FE2O4)3         95.16        63.77        .00       10.64       25.00    TO     500.00  TR-004
BI2(MOO4)3          84.91        25.69        .00       11.04       25.00    TO     500.00  TR-004
BI2(SO3)3           45.46        53.50        .00         .00       25.00    TO     500.00  TR-001

BI2(SO4)3           52.63        61.22        .00        1.74       25.00    TO     500.00  TR-001
BI2(TIO3)3          76.12        10.93        .00       10.49       25.00    TO     500.00  TR-004
BI2(V2O6)3         164.27        19.69        .00       39.64       25.00    TO     500.00  TR-004
BI2(WO4)3           91.62        13.78        .00       14.39       25.00    TO     500.00  TR-004
BO(GAS)                                                                      TO

BS(GAS)              5.96         4.73      -2.12         .00       25.00    TO     727.00  JA-001
B2O3                 8.73        25.40        .00        1.31       25.50    TO     700.00  LA-001
B2S3                14.32        22.03        .00         .67       25.00    TO     310.00  TR-009
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DATE  6  OCT.  1971        HEAT CAPACITY (CAL/GMOLE/DEG.K) CONTINUED                    PAGE:    5

                                EQUATION  CP =  A  +  BT  +  CT**2  -  D/T**2

                                COEFFICIENTS                              TEMPERATURE  RANGE       REFERENCES
   COMPOUND              A       BX10**3     CX10**6    DX10**-5         DEGREES CENTIGRADE

C                      2.90       2.49         .00        1.48          25.00    TO     727.00   JA-001
                       6.02        .04         .00        9.15         727.00    TO    1727.00
CA                     5.02       3.74         .00        -.12          25.00    TO     440.00   LA-001,PE-001
                       1.29       7.97         .00       -1.97         440.00    TO     700.00

CAAL2O4               36.00       5.96         .00        7.96          25.00    TO    1500.00   KU-001
CAAL4O7               66.09       5.48         .00       17.80          25.00    TO    1500.00   KU-001
CACO3                 24.97       5.24         .00        6.20          25.00    TO     700.00   LA-001
CACRO4                33.14       6.48         .00        6.62         227.00    TO     627.00   TR-004
CACR2O4               40.37       3.27         .00        5.40          25.00    TO     600.00   TR-004

CAFE2O4               39.39       4.76         .00        3.66          25.00    TO    1200.00   LA-001,KU-001
CAMOO3                                                                           TO
CAMOO4                31.92       6.98         .00        5.35         227.00    TO     627.00   TH-004
CAO                   11.36       1.08         .00        1.66         227.00    TO     627.00   LA-001
CAS                   10.20       3.80         .00         .00          25.00    TO     727.00   KU-001,LA-001,
                                                                                 TO              TH-009

CASO3                 18.77      16.18         .00        1.66          25.00    TO     600.00   TH-001
CASO4                 17.22      23.37         .00         .33          25.00    TO     700.00   LA-001,NB-003
CATIO3                30.47       1.36         .00        6.69          25.00    TO    1260.00   KU-001
CAV2O6                58.36       4.98         .00       14.87          25.00    TO     600.00   TH-004
CAWO4                 34.15       3.07         .00        6.47         227.00    TO     627.00   TR-004

CA(NO2)2               5.90      51.44         .00       -3.28          59.00    TO     200.00   RA-005
CA(NO3)2              29.37      36.81         .00        4.13          25.00    TO     527.00   LA-908,KE-909
CA(NO3)2.2H2O                                                                    TO
CA(NO3)2.3H2O                                                                    TO
CA(NO3)2.4H2O                                                                    TO

CA(OH)2                8.90      23.54         .00         .05            .00    TO     726.80   LA-908
CA2FE2O5              47.18      20.75         .00        6.87          25.00    TO     600.00   TH-004
CA3N2                 20.44      22.00         .00         .00          25.00    TO     527.00   LA-908,KU-903,
                                                                                 TO              KE-909
CD                     4.76       3.73         .00        -.36          25.00    TO     321.00   LA-001,PE-001
                       7.10        .00         .00         .00         321.00    TO     700.00
CDAL2O4               36.05       6.42         .00        7.92          25.00    TO     700.00   TR-004
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DATE  6  OCT.  1971        HEAT CAPACITY (CAL/GMOLE/DEG.K) CONTINUED                    PAGE:    6

                                EQUATION  CP =  A  +  BT  +  CT**2  -  D/T**2

                                COEFFICIENTS                              TEMPERATURE  RANGE       REFERENCES
   COMPOUND              A       BX10**3     CX10**6    DX10**-5         DEGREES CENTIGRADE

CDCO3                 22.70       7.94         .00        5.77          25.00    TO     700.00   TR-001
CDCRO4                30.95       7.48         .00        4.96          25.00    TO     700.00   TR-004
CDCR2O4               38.17       4.28         .00        3.74          25.00    TO     700.00   TR-004
CDFE2O4               36.10      16.83         .00        5.60          25.00    TO     700.00   TH-004
CDMOO4                29.71       7.98         .00        3.68          25.00    TO     700.00   TR-004

CDO                    9.65       2.08         .00         .00          25.00    TO     700.00   LA-001
CDS                   12.93        .87         .00         .00          25.00    TO     700.00   LA-001,KU-001
CDSO3                 16.56      17.18         .00         .00          25.00    TC     700.00   TR-001
CDSO4                 18.49      18.48         .00         .01          25.00    TO     700.00   LA-001
CDTIO3                26.78       3.06         .00        3.50          25.00    TO     700.00   TR-004

CDV2O6                58.62       2.80         .00       14.91          25.00    TO     700.00   TR-004
CDWO4                 31.94       4.01         .00        4.80          25.00    TO     700.00   TR-004
CD(NO2)2               3.69      52.44         .00       -4.94          59.00    TO     200.00   RA-005
CD(NO3)2              42.90      19.01         .00       11.06          25.00    TO     627.00   RA-005
CD(NO3)2.2H2O                                                                    TO

CD(NO3)2.4H2O                                                                    TO
CD(OH)2                                                                          TO
CD3N2                                                                            TO
CE                     5.93       3.74         .00         .10          25.00    TO     777.00   LA-001,PE-001
                       8.00        .00         .00         .00         777.00    TO    2727.00
CEN                                                                              TO

CEO2                  15.00       2.51         .00         .00          25.00    TO    1700.00   LA-001
CES                                                                              TC
CES2                  18.72        .27         .00        -.43          25.00    TO    1700.00   TR-009
CE(CO3)2              41.11      14.24         .00       11.54          25.00    TO    1700.00   TR-C01
CE(NO2)3               3.66      78.70         .00       -7.41          59.00    TO     200.00   RA-005

CE(NO2)4               3.10     103.20         .00       -9.88          59.00    TO     200.00   RA-005
CE(NO3)3              62.47      28.57         .00       16.59         300.00    TO     627.00   RA-005
CE(NO3)4              81.51      36.38         .00       22.12          25.00    TO     627.00   RA-005
CE(SO3)2              28.83      32.71         .00         .00          25.00    TO    1700.00   TR-001
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EQUATION CP = A + BT + CT**2 - D/T**2

COMPOUND	A	COEFFICIENTS BX10**3	CX10**6	DX10**-5	TEMPERATURE RANGE DEGREES CENTIGRADE			REFERENCES
CE(SO4)2	33.61	37.90	.00	1.16	25.00	TO	1700.00	TR-001
CE2O3	25.17	6.53	.00	.00	300.00	TO	840.00	CA-018
CE2S3	30.75	2.97	.00	-.64	300.00	TO	840.00	TR-009
CE2(CO3)3	64.34	25.92	.00	17.31	300.00	TO	840.00	TR-001
CE2(SO3)3	45.30	51.63	.00	.00	300.00	TO	840.00	TR-001
CE2(SO4)3	53.07	59.55	.00	1.74	300.00	TO	840.00	TR-001
CE3S4						TO		
CO	5.79	2.47	.00	.59	25.00	TO	445.00	LA-001,PE-001
	-3.17	10.46	.00	-15.73	445.00	TO	700.00	
COAL2O4	37.35	3.36	.00	7.52	25.00	TO	700.00	TR-004
COCO3	28.59	7.01	.00	5.37	25.00	TO	1200.00	TR-001
[illegible]	32.32	7.44	.00	4.56	25.00	TO	700.00	TR-004
COCR2O4	40.05	4.23	.00	3.33	25.00	TO	1200.00	TR-004
COFE2O4	30.45	31.56	.00	[illegible]	25.00	TO	500.00	LA-056
	48.27	.00	.00	.00	500.00	TO	1000.00	
COMOO4	31.59	7.94	.00	3.26	25.00	TO	700.00	TR-004
[illegible]						TO		
COO	11.53	2.94	.00	-.40	25.00	TO	1200.00	LA-001
COS	10.69	2.41	.00	.03	25.00	TO	700.00	LA-001
COSO3	16.44	17.14	.00	-.40	25.00	TO	1200.00	TR-001
COSO4	30.09	9.91	.00	.01	25.00	TO	700.00	LA-001
COTIO3	28.66	3.01	.00	3.09	25.00	TO	1200.00	TR-004
COV2O6	65.39	-3.42	.00	17.94	25.00	TO	1200.00	TR-004
COWO4	33.83	3.97	.00	4.40	25.00	TO	1200.00	TR-004
CO(NO2)2	5.58	52.40	.00	-5.34	59.00	TO	200.00	RA-005
CO(NO3)2	44.79	18.97	.00	10.66	25.00	TO	627.00	RA-005
CO(NO3)2.2H2O						TO		
CO(NO3)2.3H2O						TO		
CO(NO3)2.4H2O						TO		

EQUATION CP = A + BT + CT**2 - D/T**2

COMPOUND	A	COEFFICIENTS BX10**3	CX10**6	DX10**-5	TEMPERATURE RANGE DEGREES CENTIGRADE			REFERENCES
CO(NO3)2.6H2O						TO		
CO(OH)2						TO		
CO(OH)3						TO		
CO2	6.58	9.13	-2.65	.00	25.00	TO	1700.00	LA-001
CO2S3						TO		
CO3N						TO		
CO3O4	30.82	17.07	.00	5.76	25.00	TO	700.00	LA-001
CO3S4	38.27	12.59	.00	4.90	25.00	TO	700.00	TR-009
CR	5.84	2.35	.00	.89	25.00	TO	1200.00	LA-001,PE-001
CRN	9.84	3.90	.00	.00	.00	TO	527.00	KU-903
CRO3	21.28	5.40	.00	4.96	25.00	TO	700.00	TR-008
CR(NO2)3	5.33	76.60	.00	-5.54	59.00	TO	200.00	RA-005
CR(NO2)6	3.43	156.50	.00	-9.87	59.00	TO	200.00	RA-005
CR(NO3)3	64.15	26.50	.00	18.46	25.00	TO	627.00	RA-005
CR(NO3)6	121.05	56.20	.00	38.14	25.00	TO	627.00	RA-005
CR(OH)3						TO		
CR2N	11.01	16.40	.00	.00	25.00	TO	527.00	KE-909
CR2O3	28.52	2.20	.00	3.74	25.00	TO	1200.00	LA-001
CR2O7						TO		
CR2S3	34.12	-1.16	.00	3.10	25.00	TO	1200.00	TR-009
CR2(CO3)3	67.69	19.80	.00	21.05	25.00	TO	1200.00	TR-001
CR2(SO3)3	49.26	47.50	.00	3.74	25.00	TO	1200.00	TR-001
CR2(SO4)3	56.43	55.42	.00	5.46	25.00	TO	1200.00	TR-001
CS	7.50	.00	.00	.00	25.00	TO	28.64	LA-001,PE-001
	7.60	.00	.00	.00	28.64	TO	627.00	
CSNO2						TO		
CSNO3	21.57	55.97	.00	.00	50.00	TO	151.00	MO-912
	27.03	32.66	.00	.00	151.00	TO	405.00	
CSNO3.4H2O						TO		
CSOH						TO		

EQUATION CP = A + BT + CT**2 - D/T**2

COMPOUND	A	COEFFICIENTS BX10**3	CX10**6	DX10**-5	TEMPERATURE RANGE DEGREES CENTIGRADE			REFERENCES
CSOH.H2O						TO		
CS2AL2O4						TO		
CS2CO3						TO		
CS2CHO4						TO		
CS2CRO4						TO		
CS2FE2O4						TO		
CS2MOO4						TO		
CS2O						TO		
CS2S						TO		
CS2SO3						TO		
CS2SO4						TO		
CS2TIO3						TO		
CS2V2O6						TO		
CS2WO4						TO		
CS2(G)	8.85	8.64	-3.29	.00	25.00	TO	1200.00	LA-001
CU	5.40	1.50	.00	-.00	25.00	TO	1084.00	LA-001,PE-001
	7.50	.00	.00	.00	1084.00	TO	1200.00	
CUAL2O4	35.67	9.14	.00	7.92	25.00	TO	700.00	TR-004
CUCO3	22.32	10.66	.00	5.77	25.00	TO	700.00	TR-001
CUCRO4	30.55	10.20	.00	4.96	25.00	TO	700.00	TR-004
CUCR2O4	37.79	7.00	.00	3.74	25.00	TO	700.00	TR-004
CUFEO2	20.[illegible]7	10.23	.00	2.80	25.00	TO	700.00	TR-004
CUFE2O4	33.01	1.36	.00	1.44	25.00	TO	900.00	CA-079
CUMOO4	29.33	10.70	.00	3.68	25.00	TO	700.00	TR-004
CUNO2	4.47	28.03	.00	-2.47	59.00	TO	200.00	RA-005
CUNO3	24.07	11.32	.00	5.53	25.00	TO	627.00	RA-005
CUO	9.27	4.80	.00	.00	25.00	TO	700.00	LA-001
CUO*CUSO4	28.07	21.97	.00	.03	25.00	TO	700.00	TR-004
CUS	11.13	3.68	.00	-.22	25.00	TO	700.00	TR-009,KE-002

EQUATION CP = A + BT + CT**2 - D/T**2

COMPOUND	A	COEFFICIENTS BX10**3	CX10**6	DX10**-5	TEMPERATURE RANGE DEGREES CENTIGRADE			REFERENCES
CUSO3	16.18	19.90	.00	.00	25.00	TO	700.00	TR-001
CUSO4	18.80	17.18	.00	.03	25.00	TO	600.00	LA-001
CUTIO3	26.40	5.73	.00	3.50	25.00	TO	700.00	TR-004
CUVO3	31.93	3.21	.00	7.45	25.00	TO	700.00	TR-004
CUV2O6	58.24	5.52	.00	14.91	25.00	TO	700.00	TR-004
CUWO4	31.56	6.73	.00	4.80	25.00	TO	700.00	TR-004
CU(NO2)2	3.32	55.16	.00	-4.94	59.00	TO	200.00	RA-005
CU(NO3)2	42.53	21.73	.00	11.06	25.00	TO	627.00	RA-005
CU(NO3)2.3H2O						TO		
CU(NO3)2.6H2O						TO		
CU(OH)2	13.71	17.86	.00	-5.99	24.84	TO	160.00	ST-918
	29.11	.53	.00	12.00	160.00	TO	1227.00	
CU2AL2O4	41.30	10.04	.00	7.92	25.00	TO	700.00	TR-004
CU2CO3	27.95	11.56	.00	5.77	25.00	TO	700.00	TR-001
CU2CRO4	36.18	11.10	.00	4.96	25.00	TO	700.00	TR-004
CU2CR2O4	43.42	7.90	.00	3.74	25.00	TO	700.00	TR-004
CU2MOO4	34.95	11.60	.00	3.68	25.00	TO	700.00	TR-004
CU2O	14.89	5.70	.00	.00	25.00	TO	700.00	LA-001
CU2S	19.49	.00	.00	.00	25.00	TO	103.00	LA-001
	23.24	.00	.00	.00	103.00	TO	350.00	
	20.31	.00	.00	.00	350.00	TO	700.00	
CU2SO3	21.80	20.80	.00	.00	25.00	TO	700.00	TR-001
CU2SO4	24.19	23.40	.00	.58	25.00	TO	700.00	TR-001
CU2TIO3	32.02	6.68	.00	3.50	25.00	TO	700.00	TR-004
CU2WO4	37.19	7.63	.00	4.80	25.00	TO	700.00	TR-004
CU3N						TO		
C(D)	6.31	1.96	-.38	.00	25.00	TO	1700.00	LA-001
FE	4.13	6.38	.00	.00	.00	TO	760.00	PE-001
FEAL2O4	38.05	6.34	.00	8.68	25.00	TO	700.00	TR-004
FECO3	11.62	26.78	.00	.00	25.00	TO	500.00	LA-001

EQUATION CP = A + BT + CT**2 - D/T**2

COMPOUND		COEFFICIENTS			TEMPERATURE RANGE			REFERENCES
	A	BX10**3	CX10**6	DX10**-5	DEGREES CENTIGRADE			
FECRO4	32.94	7.40	.00	5.72	25.00	TO	700.00	TR-004
FECR2O4	38.96	5.34	.00	7.62	25.00	TO	1500.00	LA-001,KU-001
FEMOO4	31.72	7.90	.00	4.44	25.00	TO	700.00	TR-004
FEO	11.66	2.00	.00	.76	25.00	TO	1200.00	LA-001
FES	5.19	26.40	.00	.00	25.00	TO	138.00	KU-001,LA-001
	17.40	.00	.00	.00	138.00	TO	325.00	
	12.20	2.38	.00	.00	325.00	TO	1195.00	
FESO3	18.57	17.10	.00	.76	25.00	TO	1200.00	TR-001
FESO4	20.96	19.74	.00	1.34	25.00	TO	1200.00	TR-001
FES2	18.00	1.18	.00	3.12	25.00	TO	700.00	LA-001,KU-001
FETIO3	27.87	4.36	.00	4.79	25.00	TO	1370.00	LA-001,KU-001
FEV2O6	65.51	-3.46	.00	19.09	25.00	TO	1200.00	TR-004
FEWO4	33.95	3.93	.00	5.56	25.00	TO	1200.00	TR-004
FE(NO2)2	5.70	52.36	.00	-4.18	59.00	TO	200.00	RA-005
FE(NO2)3	12.95	72.40	.00	1.79	59.00	TO	200.00	RA-005
FE(NO3)2	44.91	18.93	.00	11.82	25.00	TO	627.00	RA-005
FE(NO3)2.6H2O						TO		
FE(NO3)3	71.77	22.27	.00	25.80	25.00	TO	627.00	RA-005
FE(NO3)3.9H2O						TO		
FE(OH)2	26.13	3.14	.00	3.69	24.84	TO	1227.00	ST-918
FE(OH)3	31.74	7.80	.00	9.04	24.84	TO	1227.00	ST-918
FE2N	14.91	6.09	.00	.00	25.00	TO	727.00	KU-903,KE-909,
						TO		LA-908
FE2C3	23.48	18.59	.00	3.55	25.00	TO	677.00	LA-001
	35.36	.00	.00	.00	677.00	TO	767.00	
	31.70	1.76	.00	.00	767.00	TO	1200.00	
FE2TIO4	40.44	4.98	.00	5.02	25.00	TO	1200.00	TR-004
FE2TIO5	40.61	19.57	.00	7.04	25.00	TO	677.00	TR-004
FE2(AL2O4)3	105.67	27.77	.00	29.37	25.00	TO	700.00	TR-004
FE2(CO3)3	82.93	11.33	.00	35.72	25.00	TO	1200.00	TR-001
FE2(CRO4)3	90.31	30.45	.00	20.47	25.00	TO	700.00	TR-004

EQUATION CP = A + BT + CT**2 - D/T**2

COMPOUND		COEFFICIENTS			TEMPERATURE RANGE			REFERENCES
	A	BX10**3	CX10**6	DX10**-5	DEGREES CENTIGRADE			
FE2(CR2O4)3	129.34	.33	.00	29.63	25.00	TO	1200.00	TR-004
FE2(MOO4)3	86.64	32.45	.00	16.64	25.00	TO	700.00	TR-004
FE2(SO3)3	44.21	63.89	.00	3.55	25.00	TO	677.00	TR-001
FE2(SO4)3	51.38	71.41	.00	5.29	25.00	TO	600.00	TR-001
FE2(TIO3)3	95.16	-3.33	.00	28.90	25.00	TO	1200.00	TR-004
FE2(V2O6)3	205.32	-22.64	.00	73.42	25.00	TO	1200.00	TR-004
FE2(WO4)3	110.65	-.47	.00	32.80	25.00	TO	1200.00	TR-004
FE3O4	21.87	48.19	.00	.00	25.00	TO	627.00	LA-001
	47.97	.00	.00	.00	627.00	TO	1200.00	
FE4N	26.84	8.16	.00	.00	25.00	TO	727.00	LA-908
GA	6.23	.00	.00	.00	25.00	TO	29.78	LA-001
	6.64	.00	.00	.00	29.78	TO	700.00	
GAN						TO		
GAS						TO		
GA(NO2)3	-3.05	88.10	.00	-7.41	59.00	TO	200.00	RA-005
GA(NO3)3	55.77	37.99	.00	16.59	25.00	TO	600.00	RA-005
GA(OH)3						TO		
GA2O3	11.77	25.18	.00	.00	25.00	TO	600.00	LA-001
GA2S3	17.34	21.82	.00	-.64	25.00	TO	600.00	TR-009
GA2(CO3)3	50.93	42.76	.00	17.31	25.00	TO	600.00	TR-001
GA2(SO3)3	32.50	70.48	.00	.00	25.00	TO	600.00	TR-001
GA2(SO4)3	39.67	78.40	.00	1.74	25.00	TO	600.00	TR-001
GE	5.94	.88	.00	.54	25.00	TO	937.20	LA-001
	7.00	.00	.00	.00	937.20	TO	1200.00	
GEO(GAS)						TO		
GEO2	11.19	7.17	.00	.00	25.00	TO	707.00	LA-001
GES	10.66	3.72	.00	.00	25.00	TO	1700.00	CA-072
GES2	14.14	6.25	.00	.00	25.00	TO	825.00	CA-072
GE(CO3)2	37.31	18.90	.00	11.54	25.00	TO	707.00	TR-001
GE(SO3)	25.02	37.37	.00	.00	25.00	TO	700.00	TR-001

EWUATION CP = A + BT + CT**2 - D/T**2

COMPOUND	COEFFICIENTS A	BX10**3	CX10**6	DX10**-5	TEMPERATURE RANGE DEGREES CENTIGRADE			REFERENCES
GE(SO4)2	29.80	42.65	.00	1.16	25.00	TO	700.00	TR-001
GE3N4						TO		
HF	5.73	1.19	.00	-.00	25.00	TO	1200.00	LA-001
HFN	9.84	2.22	.00	.00	25.00	TO	1727.00	KE-909
HFO2	17.38	2.08	.00	3.48	25.00	TO	1200.00	LA-001
HFS2	21.11	-.16	.00	3.05	25.00	TO	1200.00	TR-009
HF(CO3)2	43.49	13.81	.00	15.02	25.00	TO	1200.00	TR-001
HF(NO2)4	5.48	102.80	.00	-6.41	59.00	TO	200.00	RA-005
HF(NO3)4	83.89	35.95	.00	25.60	25.00	TO	627.00	RA-005
HF(SO3)2	31.20	32.28	.00	3.48	25.00	TO	1200.00	TR-001
HF(SO4)2	35.98	37.56	.00	4.64	25.00	TO	1200.00	TR-001
H2	6.94	-.19	.47	.00	25.00	TO	1200.00	JA-001
H2O(GAS)	6.78	3.57	-.46	.00	25.00	TO	2700.00	LA-001
IR	5.56	1.42	.00	.00	25.00	TO	1200.00	LA-001,PE-001
IRO2	9.17	15.19	.00	.00	25.00	TO	700.00	LA-001
IRS2	12.89	12.95	.00	-.43	25.00	TO	700.00	TR-009,WE-001
IRS3						TO		
IR(SO4)2	27.77	50.68	.00	1.16	25.00	TO	700.00	TR-001
IR2S3						TO		
K	7.16	.00	.00	.00	25.00	TO	63.20	LA-001
	8.91	-4.64	2.99	.00	63.20	TO	700.00	
KALO2	22.16	6.83	.00	4.16	25.00	TO	700.00	TR-004
KFEO2	29.84	2.67	.00	8.62	25.00	TO	900.00	TR-004
KNO2	5.98	29.84	.00	-2.27	59.00	TO	200.00	RA-005
KNO3	14.55	28.39	.00	.00	25.00	TO	127.90	LA-908
	28.80	.00	.00	.00	127.90	TO	334.30	
	29.49	.00	.00	.00	334.30	TO	427.00	
KOH	2.07	38.79	.00	-.31	.00	TO	249.00	ST-917
	18.80	.00	.00	.00	249.00	TC	1227.00	
KOH.H2O						TO		

EWUATION CP = A + BT + CT**2 - D/T**2

COMPOUND	COEFFICIENTS A	BX10**3	CX10**6	DX10**-5	TEMPERATURE RANGE DEGREES CENTIGRADE			REFERENCES
KOH.0.75H2O						TO		
KOH.2H2O						TO		
KVO3	36.23	1.57	.00	9.68	25.00	TO	900.00	TR-004
K2CO3	30.97	15.19	.00	6.17	25.00	TO	900.00	JA-001
K2CRO4	39.19	14.72	.00	5.36	25.00	TO	700.00	TR-004
K2CR2O4	46.43	11.52	.00	4.14	25.00	TO	900.00	TR-004
K2MOO4	37.97	15.22	.00	4.08	25.00	TO	700.00	TR-004
K2O	17.91	9.32	.00	.40	25.00	TO	900.00	LA-001
K2S	16.78	4.74	.00	.00	25.00	TO	547.00	DW-001
K2SO3	24.82	24.42	.00	.40	25.00	TO	1200.00	TR-001
K2SO4	28.76	23.79	.00	4.26	25.00	TO	595.00	LA-001
	33.59	13.40	.00	.00	595.00	TC	1069.00	
	47.78	.00	.00	.00	1069.00	TO	1200.00	
K2TIO3	35.04	10.30	.00	3.90	25.00	TO	900.00	TR-004
K2WO4	40.21	11.25	.00	5.20	25.00	TO	900.00	TR-004
LA	6.17	1.60	.00	.00	25.00	TO	548.00	LA-001,PE-001
LAN						TO		
LAS						TO		
LAS2						TO		
LA(NO2)3	5.50	77.10	.00	-5.78	59.00	TO	200.00	RA-005
LA(NO3)3	64.31	26.94	.00	18.23	25.00	TO	627.00	RA-005
LA(NO3)3.6H2O						TO		
LA2O3	28.86	3.07	.00	3.27	25.00	TO	700.00	NB-003,LA-001
LA2S3	34.44	-.29	.00	2.62	25.00	TO	700.00	TR-009
LA2(CO3)3	68.03	20.67	.00	20.58	25.00	TO	700.00	TR-001
LA2(SO3)3	49.59	48.37	.00	3.27	25.00	TO	700.00	TR-001
LA2(SO4)3	56.76	56.29	.00	5.01	25.00	TO	700.00	TR-001
LI	5.11	4.47	.00	.52	25.00	TO	180.50	LA-001
	8.46	-3.51	1.96	.00	180.50	TO	700.00	
LIALO2	20.66	5.21	.00	5.65	25.00	TO	700.00	TR-004

DATE 6 OCT. 1971

HEAT CAPACITY (CAL/GMOLE/DEG.K) CONTINUED

EQUATION CP = A + BT + CT**2 - D/T**2

COMPOUND	A	COEFFICIENTS BX10**3	CX10**6	DX10**-5	TEMPERATURE RANGE DEGREES CENTIGRADE			REFERENCES
LIFEO2	20.69	10.42	.00	4.49	25.00	TO	700.00	TR-004
LINO2	4.49	28.22	.00	-.78	59.00	TO	200.00	RA-005
LINO3	14.98	21.20	.00	.00	25.00	TO	253.00	LA-908
	26.60	.00	.00	.00	253.00	TO	427.00	
LINO3.3H2O						TO		
LIOH	2.99	23.75	.00	.11	.00	TO	471.30	ST-917
	17.53	2.87	.00	10.63	471.30	TO	1727.00	
LI[illegible].H2O	4.23	50.84	.00	.28	.00	TO	24.99	LA-908
LIV[illegible]	31.95	3.40	.00	9.14	25.00	TO	700.00	TR-004
LI2CO3	5.04	49.66	.00	-2.85	25.00	TO	410.00	JA-001
	4.30	42.42	.00	1.35	410.00	TO	720.00	
LI2CRO4	36.22	11.48	.00	8.33	25.00	TO	700.00	TR-004
LI2CR2O4	43.46	8.28	.00	7.12	25.00	TO	700.00	TR-004
LI2MOO4	34.99	11.98	.00	7.06	25.00	TO	700.00	TR-004
LI2O	14.93	6.08	.00	3.38	25.00	TO	700.00	LA-001
LI2S	16.79	4.96	.00	3.16	25.00	TO	700.00	TR-009
LI2SO3	21.84	21.18	.00	3.38	25.00	TO	700.00	TR-001
LI2SO4	24.23	23.82	.00	3.96	25.00	TO	700.00	TR-001
LI2TIO3	32.06	7.06	.00	6.88	25.00	TO	700.00	TR-004
LI2WO4	37.23	8.01	.00	8.17	25.00	TO	700.00	TR-004
LI3N	27.71	3.92	.00	10.13	24.84	TO	1727.00	ST-918
MG	5.52	2.33	.00	.30	25.00	TO	649.50	LA-001,PE-001
	8.10	.00	.00	.00	649.50	TO	727.00	
MGAL2O4	36.80	6.40	.00	9.78	25.00	TO	1500.00	KU-001
MGCO3	18.61	13.79	.00	4.16	25.00	TO	427.00	JA-001,LA-001
MGCRO4	31.46	7.14	.00	6.44	25.00	TO	700.00	TR-004
MGCR2O4	40.20	3.56	.00	9.58	25.00	TO	1500.00	KU-001
MGFE2O4	21.05	44.55	.00	.00	25.00	TO	392.00	LA-001
	45.39	.00	.00	.00	392.00	TO	957.00	
	25.66	13.57	.00	.00	957.00	TO	1750.00	
MGMOO4	25.19	12.60	.00	.00	25.00	TO	827.00	CA-076

DATE 6 OCT. 1971

HEAT CAPACITY (CAL/GMOLE/DEG.K) CONTINUED

EQUATION CP = A + BT + CT**2 - D/T**2

COMPOUND	A	COEFFICIENTS BX10**3	CX10**6	DX10**-5	TEMPERATURE RANGE DEGREES CENTIGRADE			REFERENCES
MGO	10.17	1.74	.00	1.48	25.00	TO	1727.00	LA-001
MGS	9.24	2.50	.00	-.01	25.00	TO	700.00	JA-001
MGSO3	17.09	16.84	.00	1.48	25.00	TO	700.00	TR-001
MGSO4	16.53	21.80	.00	.02	25.00	TO	1127.00	JA-001
MGTIO3	28.29	3.28	.00	6.53	25.00	TO	1500.00	KU-001,LA-001
MGTI2O5	44.43	3.70	.00	8.46	25.00	TO	1200.00	TR-004
MGV2O6	64.03	-3.72	.00	19.81	25.00	TO	1200.00	TR-004
MGWO4	32.47	3.67	.00	6.27	25.00	TO	1200.00	TR-004
MG(NO2)2	4.22	52.10	.00	-3.46	59.00	TO	200.00	RA-005
MG(NO3)2	10.68	71.20	.00	-1.79	25.00	TO	327.00	LA-908,KE-909
MG(NO3)2.2H2O						TO		
MG(NO3)2.6H2O						TO		
MG(OH)2	2.12	48.44	.00	.10	.00	TO	226.80	ST-918
	16.59	15.39	.00	1.84	226.80	TO	726.80	
MG2TIO4	35.96	8.54	.00	6.89	25.00	TO	1545.00	KE-002
MG3N2	20.77	11.20	.00	.00	25.00	TO	550.00	KU-903,KE-909
	20.07	10.66	.00	.00	550.00	TO	788.00	
	28.50	.00	.00	.00	788.00	TO	1027.00	
MN	3.76	7.47	.00	.00	.00	TO	825.00	PE-001
MNAL2O4	37.50	6.26	.00	8.80	25.00	TO	700.00	TR-004
MNCO3	21.99	9.30	.00	4.69	25.00	TO	427.00	LA-001,KE-002
MNCRO4	32.39	7.34	.00	5.84	25.00	TO	700.00	TR-004
MNCR2O4	39.63	4.14	.00	4.62	25.00	TO	1200.00	TR-004
MNFE2O4	54.87	-4.32	.00	19.29	25.00	TO	1200.00	TR-004
MNMOO4	31.12	7.83	.00	4.56	25.00	TO	700.00	TR-004
MNO	11.10	1.94	.00	.88	25.00	TO	1200.00	LA-001
MNO2	16.59	2.44	.00	3.88	25.00	TO	500.00	LA-001
MNS	11.40	1.80	.00	.00	25.00	TO	1200.00	LA-001
MNSO3	18.01	17.04	.00	.88	25.00	TO	1200.00	TR-001
MNSO4	29.24	8.92	.00	7.04	25.00	TO	700.00	LA-001

EQUATION CP = A + BT + CT**2 - D/T**2

COMPOUND		COEFFICIENTS			TEMPERATURE RANGE			REFERENCES
	A	BX10**3	CX10**6	DX10**-5	DEGREES CENTIGRADE			
MNS2	20.31	.20	.00	3.44	25.00	TO	500.00	TR-009
MNTIO3	28.24	2.92	.00	4.38	25.00	TO	1200.00	TR-004
MNV206	64.96	-3.52	.00	19.21	25.00	TO	1200.00	TR-004
MNWO4	33.39	3.87	.00	5.68	25.00	TO	1200.00	TR-004
MN(NO2)2	5.15	52.30	.00	-4.06	59.00	TO	200.00	RA-005
MN(NO2)3	3.43	79.70	.00	-5.80	59.00	TO	200.00	RA-005
MN(NO2)4	4.69	103.20	.00	-6.01	59.00	TO	200.00	RA-005
MN(NO3)2	44.36	18.87	.00	11.94	25.00	TO	627.00	RA-005
MN(NO3)2,3H20						TO		
MN(NO3)2,4H20						TO		
MN(NO3)2,6H20	102.59	148.10	.00	.00	25.00	TO	127.00	MA-925
MN(NO3)3	62.25	29.59	.00	18.21	25.00	TO	627.00	RA-005
MN(NO3)4	83.10	36.31	.00	26.00	25.00	TO	500.00	RA-005
MN(OH)2						TO		
MN(OH)3						TO		
MN(SO4)2	35.19	37.92	.00	5.04	25.00	TO	500.00	TR-001
MN203	24.73	8.38	.00	3.23	25.00	TO	700.00	LA-001
MN2(AL204)3	103.94	21.40	.00	27.00	25.00	TO	700.00	TR-004
MN2(CO3)3	63.89	25.97	.00	20.54	25.00	TO	700.00	TR-001
MN2(CRO4)3	88.58	24.57	.00	18.10	25.00	TO	700.00	TR-004
MN2(CR204)3	110.30	14.97	.00	14.44	25.00	TO	700.00	TR-004
MN2(FE204)3	104.10	52.64	.00	20.04	25.00	TO	700.00	TR-004
MN2(MOO4)3	84.91	26.07	.00	14.26	25.00	TO	700.00	TR-004
MN2(SO3)3	45.46	53.68	.00	3.23	25.00	TO	700.00	TR-001
MN2(SO4)3	52.63	61.60	.00	4.97	25.00	TO	700.00	TR-001
MN2(TIO3)3	76.12	11.31	.00	13.72	25.00	TO	700.00	TR-004
MN2(V206)3	171.64	10.55	.00	47.95	25.00	TO	700.00	TR-004
MN2(WO4)3	91.62	14.16	.00	17.62	25.00	TO	700.00	TR-004
MN3N2	22.32	22.40	.00	.00	25.00	TO	527.00	KE-909,LA-908

EQUATION CP = A + BT + CT**2 - D/T**2

COMPOUND		COEFFICIENTS			TEMPERATURE RANGE			REFERENCES
	A	BX10**3	CX10**6	DX10**-5	DEGREES CENTIGRADE			
MN3O4	34.62	10.82	.00	2.20	25.00	TO	1172.00	LA-001
	50.17	.00	.00	.00	1172.00	TO	1227.00	
MN4N	21.15	30.50	.00	.00	25.00	TO	527.00	KE-909
MN5N2	30.55	38.40	.00	.00	25.00	TO	527.00	KE-909,KU-903
MN8N2	42.30	60.99	.00	.00	25.00	TO	527.00	LA-908
MO	5.31	1.49	.00	-.00	25.00	TO	1200.00	LA-001,PE-001
MOO2						TO		
MOO3	20.06	5.90	.00	3.68	25.00	TO	700.00	LA-001
MOS2	11.20	13.50	.00	.00	25.00	TO	450.00	KE-002
MOS3	25.64	2.54	.00	3.03	25.00	TO	700.00	TR-009
MO(CO3)3	59.23	23.50	.00	20.99	25.00	TO	700.00	TR-001
MO(SO3)3	40.79	51.20	.00	3.68	25.00	TO	700.00	TR-001
MO(SO4)3	47.96	59.12	.00	5.42	25.00	TO	700.00	TR-001
MO2N	11.19	13.80	.00	.00	25.00	TO	527.00	KE-909,LA-908,
						TO		KU-903
MO2S3						TO		
NA	6.74	.00	.00	.00	25.00	TO	97.82	LA-001
	9.08	-5.02	2.87	.00	97.82	TO	700.00	
NAALO2	21.05	4.87	.00	3.96	25.00	TO	700.00	TR-004
NACL	9.88	5.42	.00	-.54	25.00	TO	727.00	JA-001
NAFEO2	21.08	10.08	.00	2.80	25.00	TO	700.00	TR-004
NANO2	4.85	27.92	.00	-2.49	59.00	TO	200.00	NO-905
NANO3	6.34	53.32	.00	.00	25.00	TO	276.20	KE-909
	35.70	.00	.00	.00	276.20	TO	306.20	
	37.00	.00	.00	.00	306.20	TO	427.00	
NAOH	1.80	35.97	.00	-.20	.00	TO	292.95	ST-917
	20.56	.00	.00	.00	292.95	TO	1727.00	
NAOH.H20						TO		
NAOH.2H20						TO		
NAOH.3H20						TO		
NAOH.3.5H20						TO		

EQUATION CP = A + BT + CT**2 - D/T**2

COMPOUND	A	COEFFICIENTS BX10**3	CX10**6	DX10**-5	TEMPERATURE RANGE DEGREES CENTIGRADE			REFERENCES
NAOH.4H2O						TO		
NAOH.5H2O						TO		
NAOH.7H2O						TO		
NAVO3	32.33	3.06	.00	7.45	25.00	TO	700.00	TR-004
NA2CO3	2.63	58.33	.00	-5.85	25.00	TO	486.00	LA-001,JA-001
	12.08	30.68	.00	1.27	486.00	TO	854.00	
NA2CRO4	36.98	10.80	.00	4.96	25.00	TO	700.00	TR-004
NA2CR2O4	44.22	7.59	.00	3.74	25.00	TO	700.00	TR-004
NA2MOO4	35.75	11.28	.00	3.68	25.00	TO	700.00	TR-004
NA2MO2O7	55.79	17.17	.00	7.36	25.00	TO	700.00	TR-004
NA2O	15.69	5.40	.00	.00	25.00	TO	700.00	LA-001
NA2S	17.55	4.28	.00	-.22	25.00	TO	700.00	KE-002
NA2SO3	22.60	20.50	.00	.00	25.00	TO	700.00	LA-001,CA-004
NA2SO4	15.53	52.77	.00	.00	25.00	TO	259.00	LA-001
	29.05	19.33	.00	.00	259.00	TO	884.00	
	47.16	.00	.00	.00	884.00	TO	1200.00	
NA2TIO3	25.18	20.72	.00	.00	25.00	TO	287.00	KU-001,LA-001
	25.95	17.00	.00	.00	287.00	TO	1100.00	
NA2TI2O5	49.32	7.06	.00	4.60	25.00	TO	1000.00	KU-001
NA2TI3O7	63.46	10.64	.00	5.64	25.00	TO	1100.00	KU-001
NA2WO4	37.99	7.33	.00	4.80	25.00	TO	700.00	TR-004
NA2W2O7	60.28	9.25	.00	9.59	25.00	TO	700.00	TR-004
NB	5.66	.96	.00	-.00	25.00	TO	1200.00	LA-001
NBO						TO		
NBO2						TO		
NB2O5	36.22	5.54	.00	4.88	25.00	TO	1200.00	LA-001
NB2S5	45.53	-.07	.00	3.81	25.00	TO	1200.00	TR-009
NB2(CO3)5	101.49	34.87	.00	33.73	25.00	TO	1200.00	TR-001
NB2(SO3)5	70.77	81.04	.00	4.88	25.00	TO	1200.00	TR-001
NB2(SO4)5	82.72	94.24	.00	7.78	25.00	TO	1200.00	TR-001

EQUATION CP = A + BT + CT**2 - D/T**2

COMPOUND	A	COEFFICIENTS BX10**3	CX10**6	DX10**-5	TEMPERATURE RANGE DEGREES CENTIGRADE			REFERENCES
NI	4.11	6.95	.00	.02	25.00	TO	357.20	LA-001,PE-001
	6.00	1.80	.00	-.01	357.20	TO	1200.00	
NIAL2O4	43.33	.23	.00	12.40	25.00	TO	700.00	TR-004
NICO3	25.87	6.57	.00	7.06	25.00	TO	1200.00	TR-001
NICRO4	38.21	1.29	.00	9.43	25.00	TO	700.00	TR-004
NICR2O4	41.34	2.90	.00	5.05	25.00	TO	1200.00	TR-004
NIFE2O4	31.62	26.25	.00	4.66	25.00	TO	582.00	CA-056
	48.66	.00	.00	.00	582.00	TO	1000.00	
NIMOO4	36.98	1.79	.00	8.16	25.00	TO	700.00	TR-004
NIO	-4.99	37.56	.00	-3.89	25.00	TO	250.00	LA-001
	11.18	2.02	.00	.00	250.00	TO	1200.00	
NIS	9.25	12.80	.00	.00	25.00	TO	327.00	LA-001,KU-001
NISO3	27.69	7.28	.00	-.58	25.00	TO	700.00	TR-001
NISO4	30.08	9.92	.00	.00	25.00	TO	700.00	LA-001
NITIO3	29.95	1.68	.00	4.81	25.00	TO	1200.00	TR-004
NIV2O6	66.67	-4.76	.00	19.65	25.00	TO	1200.00	TR-004
NIWO4	35.11	2.63	.00	6.11	25.00	TO	1200.00	TR-004
NI(NO2)2	6.86	51.06	.00	-3.63	59.00	TO	200.00	RA-005
NI(NO3)2	46.07	17.64	.00	12.37	25.00	TO	627.00	RA-005
NI(NO3)2.3H2O						TO		
NI(NO3)2.6H2O						TO		
NI(OH)2						TO		
NI(OH)3						TO		
NI3N						TO		
NI3S2						TO		
NO(G)	7.03	.92	.00	.14	25.00	TO	2227.00	KE-909
NO2(G)	10.07	2.28	.00	1.67	25.00	TO	1727.00	KE-909
N2O3(G)	20.50	2.05	.00	5.14	25.00	TO	1827.00	ST-906
N2O4(G)	26.09	2.72	.00	7.95	24.84	TO	1827.00	ST-906
N2O5	12.29	36.00	.00	.00	25.00	TO	32.40	ST-906

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                                   EQUATION  CP =  A  +  BT  +  CT**2  -  D/T**2

      COMPOUND                        COEFFICIENTS                            TEMPERATURE  RANGE       REFERENCES
                           A         BX10**3     CX10**6    DX10**-5      DEGREES CENTIGRADE

   N2O5(G)               34.24          .79         .00        13.40         32.40     TO     1727.00  ST-906

   N2(GAS)                6.30         1.83        -.33          .00         25.00     TO     1727.00  JA-001
   O2                     6.53         2.06        -.36          .00         25.00     TO     2700.00  LA-001
   PB                     5.67         2.26         .00          .02         25.00     TO      327.40  LA-001,PE-001
                          7.86          .94         .21          .00        327.40     TO      700.00
   PBAL2O4               37.06         8.34         .00         7.92         25.00     TO      600.00  TR-004
   PBCO3                 23.65         9.87         .00         5.77         25.00     TO      600.00  TR-001

   PBCO3*PBO                                                                           TO
   PBCO3*2PBO                                                                          TO
   PBCRO4                31.88         9.40         .00         4.96         25.00     TO      600.00  TR-004
   PBCR2O4               39.12         6.20         .00         3.74         25.00     TO      600.00  TR-004
   PBFE2O4               34.07        22.59         .00         3.55         25.00     TO      600.00  TR-004

   PBMOO4                30.66         9.90         .00         3.68         25.00     TO      600.00  TR-004
   PBO                   10.60         4.00         .00          .00         25.00     TO      600.00  LA-001
   PBO*PBSO4             21.55        35.01         .00        -4.20         25.00     TO      600.00  TR-004
   PBO2                  12.70         7.80         .00          .00         25.00     TO      700.00  LA-001
   PBS                   10.66         5.92         .00          .00         25.00     TO      600.00  KU-001,LA-001

   PBSO3                 17.51        19.10         .00          .00         25.00     TO      600.00  TR-001
   PBSO4                 10.94        31.01         .00        -4.20         25.00     TO      700.00  LA-001
   PBTIO3                18.70        23.30         .00          .00         27.00     TO      600.00  KU-001
   PBV2O6                57.11         7.90         .00        13.21         25.00     TO      600.00  TR-004
   PBWO4                 32.89         5.93         .00         4.80         25.00     TO      600.00  TR-004

   PB(NO2)2               4.64        54.36         .00        -4.94         59.00     TO      200.00  RA-005
   PB(NO2)4                .79       108.50         .00        -9.88         59.00     TO      200.00  RA-005
   PB(NO3)2              43.85        20.93         .00        11.06         25.00     TO      600.00  RA-005
   PB(NO3)4              79.21        41.67         .00        22.12         25.00     TO      627.00  RA-005
   PB(OH)2                                                                             TO

   PB(SO4)2              31.30        43.28         .00         1.16         25.00     TO      700.00  TR-001
   PB3O4                                                                               TO
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                                   EQUATION  CP =  A  +  BT  +  CT**2  -  D/T**2

      COMPOUND                        COEFFICIENTS                            TEMPERATURE  RANGE       REFERENCES
                           A         BX10**3     CX10**6    DX10**-5      DEGREES CENTIGRADE

   PD                     5.87         1.33         .00          .14         25.00     TO     1200.00  LA-001,PE-001
   PDCO3                 16.35        20.06         .00         5.77         25.00     TO      500.00  TR-001
   PDO                    5.30        14.19         .00          .00         25.00     TO      500.00  LA-001

   PDS                    5.16        13.07         .00         -.21         25.00     TO      500.00  TR-009
   PDSO3                 10.21        29.29         .00          .00         25.00     TO      700.00  TR-001
   PDSO4                 12.60        31.95         .00          .58         25.00     TO      500.00  TR-001
   PDS2                                                                                TO
   RBNO2                                                                               TO

   RBNO3                 23.11        40.70         .00          .00         50.00     TO      160.00  MU-911
                         27.49        69.80         .00          .00        160.00     TO      220.00
                         36.06        16.50         .00          .00        220.00     TO      281.00
                         39.08          .00         .00          .00        281.00     TO      310.00
                         31.61         2.02         .00          .00        310.00     TO      350.00
   RBOH                                                                                TO
   RBOH.H2O                                                                            TO
   RBOH.2H2O                                                                           TO
   RB2CO3                28.38          .00         .00          .00         25.00     TO       26.00  LA-001

   RB2O                                                                                TO
   RB2S                                                                                TO
   RB2SO3                                                                              TO
   RB2SO4                                                                              TO
   RE                     5.66         1.30         .00         -.00         25.00     TO     1200.00  LA-001,PE-001

   REO2                                                                                TO
   REO3                                                                                TO
   RES2                                                                                TO
   RES3                                                                                TO
   RE2O7                                                                               TO

   RE2O8                                                                               TO
   RE2S7                                                                               TO
   RH                     5.49         2.06         .00          .01         25.00     TO     1200.00  LA-001,PE-001
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EQUATION CP = A + BT + CT**2 - D/T**2

COMPOUND		COEFFICIENTS			TEMPERATURE RANGE			REFERENCES
	A	BX10**3	CX10**6	DX10**-5	DEGREES CENTIGRADE			
RHCO3	22.89	11.39	.00	5.77	25.00	TO	700.00	TR-001
RHO	9.84	5.53	.00	.00	25.00	TO	700.00	LA-001
RHS	11.70	4.41	.00	-.21	25.00	TO	700.00	TR-009
RHSO3	16.75	20.63	.00	.00	25.00	TO	700.00	TR-001
RHSO4	19.40	23.27	.00	.58	25.00	TO	700.00	TR-001
RH2O	15.60	6.47	.00	.00	25.00	TO	900.00	LA-001
RH2O3	20.72	13.76	.00	.00	25.00	TO	900.00	LA-001
RH2S	17.47	5.35	.00	-.21	25.00	TO	900.00	TR-009
RH2SO4	24.90	24.21	.00	.58	25.00	TO	600.00	TR-001
RH2S3	26.31	10.42	.00	-.64	25.00	TO	900.00	TR-009
RH2(SO4)3	48.62	67.01	.00	1.74	25.00	TO	600.00	TR-001
RU	5.24	1.50	.00	-.00	25.00	TO	727.00	LA-001
	7.20	.00	.00	.00	727.00	TO	1200.00	
RUO2						TO		
RUO3(GAS)						TO		
RUO4(GAS)						TO		
RUS2						TO		
S	5.41	.00	.00	.00	25.00	TO	115.18	JA-001
	7.46	-9.84	15.74	.00	115.18	TO	444.60	
	3.39	6.86	-.00	.00	444.60	TO	1200.00	
SB	5.50	1.76	.00	.00	25.00	TO	630.90	LA-001,PE-001
	7.50	.00	.00	.00	630.90	TO	700.00	
SB2O3	19.09	17.08	.00	.00	25.00	TO	900.00	LA-001
SB2O4	22.60	16.20	.00	.00	25.00	TO	700.00	LA-001
SB2O5						TO		
SB2S3	24.20	13.20	.00	.00	25.00	TO	648.00	KU-001,KE-002
SB2(AL2O4)3	98.30	30.10	.00	23.77	25.00	TO	700.00	TR-004
SB2(CO3)3	58.25	34.68	.00	17.31	25.00	TO	900.00	TR-001
SB2(CRO4)3	82.94	33.28	.00	14.87	25.00	TO	700.00	TR-004
SB2(CR2O4)3	104.66	23.67	.00	11.22	25.00	TO	900.00	TR-004

EQUATION CP = A + BT + CT**2 - D/T**2

COMPOUND		COEFFICIENTS			TEMPERATURE RANGE			REFERENCES
	A	BX10**3	CX10**6	DX10**-5	DEGREES CENTIGRADE			
SB2(FE2O4)3	144.40	5.12	.00	50.51	25.00	TO	900.00	TR-004
SB2(MOO4)3	79.27	34.78	.00	11.04	25.00	TO	700.00	TR-004
SB2(SO3)3	39.82	62.38	.00	.00	25.00	TO	900.00	TR-001
SB2(SO4)3	46.99	70.30	.00	1.74	25.00	TO	900.00	TR-001
SB2(TIO3)3	70.48	20.02	.00	10.49	25.00	TO	900.00	TR-004
SB2(V2O6)3	182.75	-1.46	.00	56.86	25.00	TO	900.00	TR-004
SB2(WO4)3	85.98	22.87	.00	14.39	25.00	TO	900.00	TR-004
SC	6.12	1.45	.00	.43	25.00	TO	1500.00	KR-001
SC2O3	23.16	5.64	.00	.00	25.00	TO	1700.00	LA-001
SC2(CO3)3	62.32	23.24	.00	17.31	25.00	TO	1700.00	TR-001
SC2(SO3)3	43.89	50.94	.00	.00	25.00	TO	1700.00	TR-001
SC2(SO4)3	51.06	58.86	.00	1.74	25.00	TO	1700.00	TR-001
SI	5.80	.55	.00	1.09	25.00	TO	700.00	LA-001,PE-001
SIO(GAS)						TO		
SIO2	11.21	8.20	.00	2.70	25.00	TO	867.00	LA-001
	14.40	1.94	.00	.00	867.00	TO	1610.00	
SIS(GAS)	7.25	2.41	-.78	.00	25.00	TO	1700.00	JA-001
SIS2	22.80	-2.86	.00	8.60	25.00	TO	1610.00	TR-009,JA-001
SI(CO3)2	45.18	11.12	.00	20.57	25.00	TO	1610.00	TR-001
SI(SO3)2	25.03	38.40	.00	2.69	25.00	TO	867.00	TR-001
SI(SO4)2	29.81	43.68	.00	3.85	25.00	TO	867.00	TR-001
SN	4.43	6.28	.00	.00	25.00	TO	231.90	LA-001,PE-001
	7.30	.00	.00	.00	231.90	TO	700.00	
SNCO3	22.60	9.36	.00	5.77	25.00	TO	700.00	TR-001
SNO	9.55	3.50	.00	.00	25.00	TO	700.00	LA-001,NB-002
SNO2	17.65	2.40	.00	5.16	25.00	TO	1200.00	LA-001,NB-001
SNS	8.48	7.43	.00	-.95	25.00	TO	584.00	LA-001,KU-001
	9.78	3.74	.00	.00	584.00	TO	880.00	
SNSO3	16.46	18.60	.00	.00	25.00	TO	700.00	TR-001

EWUATION CP = A + BT + CT**2 - D/T**2

COMPOUND	COEFFICIENTS				TEMPERATURE RANGE			REFERENCES
	A	BX10**3	CX10**6	DX10**-5	DEGREES CENTIGRADE			
SNSO4	18.85	21.24	.00	.58	25.00	TO	700.00	TR-001
SNS2	15.51	4.20	.00	.00	25.00	TO	700.00	LA-001,KU-001
SN(AL2O4)2	70.46	11.08	.00	21.00	25.00	TO	700.00	TR-004
SN(CO3)2	43.76	14.13	.00	16.70	25.00	TO	1200.00	TR-001
SN(CRO4)2	60.22	13.20	.00	15.07	25.00	TO	700.00	TR-004
SN(CR2O4)2	74.70	6.79	.00	12.63	25.00	TO	1200.00	TR-004
SN(FE2O4)2	105.18	-10.13	.00	41.98	25.00	TO	1200.00	TR-004
SN(MOO4)2	57.77	14.19	.00	12.52	25.00	TO	700.00	TR-004
SN(NO2)2	3.59	53.86	.00	-4.94	59.00	TO	200.00	RA-005
SN(NO2)4	5.75	103.10	.00	-4.73	59.00	TO	200.00	RA-005
SN(NO3)2	42.80	20.43	.00	11.06	25.00	TO	627.00	RA-005
SN(NO3)4	84.16	36.27	.00	27.28	25.00	TO	627.00	RA-005
SN(OH)2						TO		
SN(OH)4						TO		
SN(SO3)2	31.48	32.60	.00	5.16	25.00	TO	1200.00	TR-001
SN(SO4)2	36.26	37.88	.00	6.32	25.00	TO	1200.00	TR-001
SN(TIO3)2	51.91	4.36	.00	12.15	25.00	TO	1200.00	TR-004
SN(V2O6)2	125.36	-8.52	.00	41.83	25.00	TO	1200.00	TR-004
SN(WO4)2	62.25	6.26	.00	14.75	25.00	TO	1200.00	TR-004
SO2	7.02	9.75	-3.58	.00	25.00	TO	1200.00	LA-001
SO3	6.90	20.37	-7.12	.00	25.00	TO	1200.00	LA-001
SP	5.61	1.35	.00	.01	25.00	TO	700.00	LA-001
SRAL2O4	38.73	5.46	.00	4.73	25.00	TO	700.00	TR-004
SRCO3	21.41	8.56	.00	3.39	25.00	TO	700.00	LA-001
SRCRO4	33.62	6.52	.00	6.76	25.00	TO	700.00	TR-004
SRCR2O4	40.86	3.32	.00	5.54	25.00	TO	700.00	TR-004
SRFE2O4	38.79	15.87	.00	7.41	25.00	TO	700.00	TR-004
SRMOO3						TO		
SRMOO4	32.39	7.02	.00	5.48	25.00	TO	700.00	TR-004
SRO	12.33	1.12	.00	1.81	25.00	TO	700.00	LA-001

EQUATION CP = A + BT + CT**2 - D/T**2

COMPOUND	COEFFICIENTS				TEMPERATURE RANGE			REFERENCES
	A	BX10**3	CX10**6	DX10**-5	DEGREES CENTIGRADE			
SRS	14.20	.00	.00	1.59	25.00	TO	700.00	TR-009
SRSO3	19.24	16.22	.00	1.81	25.00	TO	700.00	TR-001
SRSO4	21.79	13.30	.00	-.00	25.00	TO	1200.00	LA-001
SRTIO3	28.23	2.04	.00	4.56	25.00	TO	1500.00	LA-001,KU-001
SRV2O6	61.31	1.85	.00	16.71	25.00	TO	700.00	TR-004
SRWO4	34.62	3.05	.00	6.60	25.00	TO	700.00	TR-004
SR(NO2)2	6.38	51.48	.00	-3.14	59.00	TO	200.00	RA-005
SR(NO3)2	28.10	39.42	.00	3.58	25.00	TO	627.00	TA-913
SR(NO3)2.4H2O						TO		
SR(OH)2	7.64	33.40	.00	.00	25.00	TO	535.00	KE-909
	36.50	.00	.00	.00	535.00	TO	927.00	
SR(OH)2.H2O						TO		
SR(OH)2.8H2O						TO		
SR2TIO4	38.45	3.84	.00	4.67	25.00	TO	1500.00	KU-001,LA-001
SR3N2						TO		
S(GAS)	5.97	-1.26	.41	.00	25.00	TO	1700.00	LA-001
TA	6.28	.42	.00	.30	25.00	TO	1200.00	LA-001,PE-001
TAN	7.73	7.80	.00	.00	25.00	TO	527.00	KE-909,KU-903,
						TO		LA-908
TA2N						TO		
TA2O5	36.98	6.56	.00	5.95	25.00	TO	1200.00	LA-001
TA2S5	46.30	.95	.00	4.88	25.00	TO	1200.00	TR-009
TA2(CO3)5	102.26	35.89	.00	34.80	25.00	TO	1200.00	TR-001
TA2(SO3)5	71.53	62.06	.00	5.95	25.00	TO	1200.00	TR-001
TA2(SO4)5	83.48	95.26	.00	8.85	25.00	TO	1200.00	TR-001
TH	5.18	4.54	.00	.00	25.00	TO	1200.00	LA-001,PE-001
THO2	15.83	2.88	.00	1.60	25.00	TO	1200.00	LA-001
THS						TO		
THS2	19.55	.64	.00	1.16	25.00	TO	1200.00	TR-009
TH(AL2O4)2	68.64	11.56	.00	17.44	25.00	TO	700.00	TR-004
TH(CO3)2	41.94	14.61	.00	13.14	25.00	TO	1200.00	TR-001

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DATE  6  OCT.  1971        HEAT CAPACITY (CAL/GMOLE/DEG.K) CONTINUED                              PAGE:   27

                              EGUATION  CP =  A  +  BT  +  CT**2  -  D/T**2

                                    COEFFICIENTS                             TEMPERATURE  RANGE        REFERENCES
  COMPOUND               A          BX10**3     CX10**6   DX10**-5           DEGREES CENTIGRADE

TH(CRO4)2              58.40         13.68        .00       11.51        25.00    TO     700.00   TR-004

TH(CR2O4)2             72.88          7.27        .00        9.08        25.00    TO    1200.00   TR-004
TH(FE2O4)2            103.36         -9.65        .00       38.42        25.00    TO    1200.00   TR-004
TH(MOO4)2              55.95         14.68        .00        8.96        25.00    TO     700.00   TR-004
TH(SO3)2               29.65         33.08        .00        1.60        25.00    TO    1200.00   TR-001
TH(SO4)2               25.00         55.20        .00         .00        25.00    TO     637.00   CA-011

TH(TIO3)2              50.09          4.84        .00        8.59        25.00    TO    1200.00   TR-004
TH(V2O6)2             123.54         -8.04        .00       38.27        25.00    TO    1200.00   TR-004
TH(WO4)2               60.43          6.74        .00       11.19        25.00    TO    1200.00   TR-004
TH2S3                                                                             TO
TI                      6.38          1.13        .00         .69        25.00    TO    1668.00   JA-001

TICO3                  22.90         10.24        .00        7.02        25.00    TO    1200.00   TR-001
TIN                    11.91           .94        .00        2.96        25.00    TO    1727.00   LA-908,KU-903,
                                                                                  TO              KE-909
TIO                    10.56          3.60        .00        1.86        25.00    TO     991.00   LA-001
                       11.84          3.01        .00         .00       991.00    TO    1200.00
TIO2                   17.13           .98        .00        3.50        25.00    TO    1200.00   LA-001
TISO3                  17.47         18.70        .00        1.86        25.00    TO    1000.00   TR-001

TISO4                  19.86         21.34        .00        2.44        25.00    TO    1000.00   TR-001
TIS2                    8.08         27.34        .00         .00        25.00    TO     147.00   KU-001
                       14.99          5.14        .00         .00       147.00    TO     737.00
TI(NO2)2                3.89         54.73        .00       -3.69        59.00    TO     200.00   RA-005
TI(NO2)3                8.58         76.00        .00       -1.98        59.00    TO     200.00   RA-005
TI(NO2)4                5.23        101.70        .00       -6.39        59.00    TC     200.00   RA-005

TI(NO3)2               43.10         21.30        .00       12.31        25.00    TO     627.00   RA-005
TI(NO3)3               67.39         25.91        .00       22.03        25.00    TO     627.00   RA-005
TI(NO3)4               83.64         34.85        .00       25.62        25.00    TO     627.00   RA-C05
TI(SO4)2               35.73         36.46        .00        4.66        25.00    TO    1200.00   TR-001
TI2O3                   7.31         53.49        .00         .00        25.00    TO     200.00   LA-001,JA-001
                       34.66          1.30        .00       10.67       200.00    TO    1200.00
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DATE  6  OCT.  1971        HEAT CAPACITY (CAL/GMOLE/DEG.K) CONTINUED                              PAGE:   28

                              EGUATION  CP =  A  +  BT  +  CT**2  -  D/T**2

                                    COEFFICIENTS                             TEMPERATURE  RANGE        REFERENCES
  COMPOUND               A          BX10**3     CX10**6   DX10**-5           DEGREES CENTIGRADE

TI2(CO3)3              74.18         18.61        .00       28.18        25.00    TO    1200.00   TR-001
TI2(SO3)3              55.97         40.05        .00       10.96        25.00    TO    1200.00   TR-001
TI2(SO4)3              63.14         53.97        .00       12.70        25.00    TO    1200.00   TR-001
TI3O5                  35.45         29.48        .00         .00        25.00    TO     177.00   LA-001
                       41.59          8.00        .C0         .00       177.00    TO     700.00
U                       2.16          9.50        .00       -1.52        25.00    TO     662.00   LA-001,PE-001
                       10.15           .00        .00         .00       662.00    TO    1133.00
                        9.15           .00        .00         .00      1133.00    TO    1200.00

UO2                    19.19          1.62        .00        3.96        25.00    TO    1200.00   LA-001
UO2SO4                 26.90         26.00        .00         .00        25.00    TO     500.00   OW-001
UO3                    22.08          2.54        .00        2.97        25.00    TO     600.00   LA-001
US                                                                                TO
US2                    15.20          8.70        .00         .00        25.00    TO     352.00   KU-001

U(AL2O4)2              72.00         10.30        .00       19.80        25.00    TO     700.00   TR-004
U(CO3)2                45.30         13.35        .C0       15.50        25.00    TO    1200.00   TR-001
U(CRO4)2               61.76         12.42        .00       13.87        25.00    TO     700.00   TR-004
U(CR2O4)2              76.24          6.02        .00       11.43        25.00    TC    1200.00   TR-004
U(FE2O4)2             106.72        -10.91        .00       40.78        25.00    TO    1200.00   TR-004

U(MOO4)2               59.31         13.42        .00       11.31        25.00    TO     700.00   TR-004
U(SO3)2                33.01         31.82        .00        3.96        25.00    TO    1200.00   TR-001
U(SO4)2                37.79         37.10        .00        5.12        25.00    TO    1200.00   TR-C01
U(TIO3)2               53.45          3.58        .00       10.95        25.00    TO    1200.00   TR-004
U(V2O6)2              126.90         -9.30        .CC       40.63        25.00    TC    1200.00   TR-004

U(WO4)2                63.78          5.48        .00       13.55        25.00    TO    1200.00   TR-004
U2S3                                                                              TC
U3O8                   67.50          8.83        .00       11.94        25.00    TO     600.00   KU-001
V                       4.36          2.42        .00        -.28        25.00    TC    1200.00   LA-001,PE-001
VCO3                   24.37          9.06        .00        7.03        25.00    TO    1200.00   TR-001

VN                     10.94          2.10        .00        2.21        25.00    TO    1527.00   LA-908,KE-909
VO                     11.31          3.22        .00        1.26        25.00    TO    1200.00   LA-001
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EQUATION CP = A + BT + CT**2 - D/T**2

COMPOUND		COEFFICIENTS			TEMPERATURE RANGE			REFERENCES
	A	BX10**3	CX10**6	DX10**-5	DEGREES CENTIGRADE			
VOSO4	27.15	19.46	.00	4.52	72.00	TO	720.00	TR-001
VS	13.18	2.10	.00	1.04	25.00	TO	1200.00	TR-009
VSO3	18.22	18.32	.00	1.26	25.00	TO	1700.00	TR-001
VSO4	20.61	20.96	.00	1.84	25.00	TO	1200.00	TR-001
V2O3	29.34	4.76	.00	5.42	25.00	TO	1200.00	LA-001
V2O4	29.89	.00	.00	.00	25.00	TO	72.00	LA-001
	35.69	3.45	.00	7.89	72.00	TO	1200.00	
V2O5	46.51	3.90	.00	13.21	25.00	TO	670.00	LA-001,NB-003
	45.58	.00	.00	.00	670.00	TO	1200.00	
V2S3	34.93	1.40	.00	4.78	25.00	TO	1200.00	TR-009
V2S4	42.67	-.69	.00	6.15	25.00	TO	1200.00	TR-009
V2S5	63.17	-11.06	.00	17.26	25.00	TO	1200.00	TR-009
V2(CO3)3	68.50	22.36	.00	22.73	25.00	TO	1200.00	TR-001
V2(SO3)3	50.07	50.06	.00	5.42	25.00	TO	1700.00	TR-001
V2(SO4)3	57.24	57.98	.00	7.16	25.00	TO	1200.00	TR-001
W	5.85	.72	.00	.24	25.00	TO	3377.00	JA-001
WO2	15.49	3.58	.00	2.80	25.00	TO	2727.00	JA-001
WO3	20.81	3.81	.00	3.85	25.00	TO	777.00	JA-001
	20.80	2.76	.00	-.10	777.00	TO	1472.00	
	31.50	.00	.00	.00	1472.00	TO	1667.00	
WS2	21.55	-.36	.00	2.91	25.00	TO	1200.00	TR-009
W(CO3)2	41.60	15.31	.00	14.34	25.00	TO	2727.00	TR-001
W(CO3)3	57.45	23.13	.00	18.20	25.00	TO	1667.00	TR-001
W(SO3)2	31.65	32.09	.00	3.34	25.00	TO	700.00	TR-001
W(SO3)3	43.03	47.23	.00	4.80	25.00	TO	1200.00	TR-001
W(SO4)2	36.43	37.37	.00	4.50	25.00	TO	1200.00	TR-001
W(SO4)3	50.20	55.15	.00	6.54	25.00	TO	1200.00	TR-001
Y	5.59	1.90	.00	-.29	25.00	TO	1500.00	KU-001
Y2O3	29.60	1.20	.00	4.78	25.00	TO	1000.00	KU-001
Y2(CO3)3	68.77	18.80	.00	22.09	25.00	TO	1000.00	TR-001

EQUATION CP = A + BT + CT**2 - D/T**2

COMPOUND		COEFFICIENTS			TEMPERATURE RANGE			REFERENCES
	A	BX10**3	CX10**6	DX10**-5	DEGREES CENTIGRADE			
Y2(SO3)3	50.33	46.50	.00	4.78	25.00	TO	1000.00	TR-001
Y2(SO4)3	57.50	54.42	.00	6.52	25.00	TO	1000.00	TR-001
ZN	5.33	2.42	.00	-.01	25.00	TO	419.50	LA-001,PE-001
	7.48	.00	.00	.00	419.50	TO	700.00	
ZNAL2O4	38.11	5.56	.00	10.10	25.00	TO	700.00	TR-004
ZNCO3	24.76	7.08	.00	7.95	25.00	TO	1200.00	TR-001
ZNCRO4	32.99	6.62	.00	7.14	25.00	TO	700.00	TR-004
ZNCR2O4	25.49	21.69	.00	.00	25.00	TO	700.00	LA-001
ZNFE2O4	30.79	13.89	.00	.00	25.00	TO	700.00	LA-001
ZNMOO4	31.76	7.12	.00	5.86	25.00	TO	700.00	TR-004
ZNO	11.70	1.22	.00	2.18	25.00	TO	1200.00	LA-001
ZNO*2ZNSO4	45.82	42.79	.00	2.18	25.00	TO	700.00	TR-004
ZNS	12.16	1.24	.00	1.36	25.00	TO	927.00	LA-001,KU-001
ZNSO3	18.61	27.28	.00	2.18	25.00	TO	1200.00	TR-001
ZNSO4	17.06	20.79	.00	.00	25.00	TO	727.00	LA-001,NB-003
ZNTIO3	28.83	2.19	.00	5.66	25.00	TO	1200.00	TR-004
ZNV2O6	65.56	-4.24	.00	20.51	25.00	TO	1200.00	TR-004
ZNWO4	33.99	3.15	.00	6.97	25.00	TO	1200.00	TR-004
ZN(NO2)2	5.75	51.58	.00	-2.76	59.00	TO	200.00	RA-005
ZN(NO3)2	44.96	18.15	.00	13.24	25.00	TO	627.00	RA-005
ZN(NO3)2.H2O						TO		
ZN(NO3)2.2H2O						TO		
ZN(NO3)2.4H2O						TO		
ZN(NO3)2.6H2O						TO		
ZN(OH)2						TO		
ZN2TIO4	39.80	5.54	.00	7.69	25.00	TO	1500.00	LA-001,KU-001
ZN3N2	19.93	20.80	.00	.00	25.00	TO	427.00	KE-909
ZP	6.83	1.12	.00	.91	25.00	TO	862.00	KU-001
	7.27	.00	.00	.00	862.00	TO	1100.00	

HEAT CAPACITY (CAL/GMOLE/DEG.K) CONTINUED

EQUATION CP = A + BT + CT**2 - D/T**2

COMPOUND	COEFFICIENTS A	BX10**3	CX10**6	DX10**-5	TEMPERATURE RANGE DEGREES CENTIGRADE			REFERENCES
ZRN	11.10	1.68	.00	1.72	25.00	TO	1427.00	KE-909,KU-903,
						TO		LA-908
ZRO2	16.63	1.80	.00	3.36	25.00	TO	700.00	LA-001
ZRS2	20.35	-.44	.00	2.92	25.00	TO	700.00	TR-009
ZR(AL2O4)2	69.44	10.48	.00	19.20	25.00	TO	700.00	TR-004
ZR(CO3)2	42.74	13.53	.00	14.90	25.00	TO	700.00	TR-001
ZR(CRO4)2	59.20	12.60	.00	13.27	25.00	TO	700.00	TR-004
ZR(CR2O4)2	73.68	6.19	.00	10.84	25.00	TO	700.00	TR-004
ZR(FE2O4)2	69.55	31.31	.00	14.57	25.00	TO	700.00	TR-004
ZR(MOO4)2	56.75	13.60	.00	10.72	25.00	TO	700.00	TR-004
ZR(NO2)2						TO		
ZR(NO2)4	4.73	102.50	.00	-6.53	59.00	TO	200.00	RA-005
ZR(NO3)2						TO		
ZR(NO3)2.6H2O						TO		
ZR(NO3)4	83.14	35.67	.00	25.48	25.00	TO	627.00	RA-005
ZR(OH)4						TO		
ZR(OH)4.H2O						TO		
ZR(OH)4.2H2O						TO		
ZR(SO3)2	30.45	32.00	.00	3.36	25.00	TO	700.00	TR-001
ZR(SO4)2	35.23	37.28	.00	4.52	25.00	TO	700.00	TR-001
ZR(TIO3)2	50.89	3.76	.00	10.35	25.00	TO	700.00	TR-004
ZR(V2O6)2	114.58	3.25	.00	33.17	25.00	TO	700.00	TR-004
ZR(WO4)2	61.23	5.66	.00	12.95	25.00	TO	700.00	TR-004
ZR3N2	21.64	26.00	.00	.00	25.00	TO	527.00	LA-908,KE-909

Radian Corporation
8500 SHOALCREEK BLVD. • AUSTIN, TEXAS 78758 • TELEPHONE 512-454-9535

TECHNICAL NOTE 200-007-06

HIGH TEMPERATURE BEHAVIOR OF ANHYDROUS AND HYDRATED NITRITE AND NITRATES

13 August 1971

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1.0 INTRODUCTION

This technical note presents the results of a literature review on the high temperature behavior of metal nitrates and nitrites. The findings of the review are discussed in terms of their implications for the use of thermal decomposition as a regeneration method in a nitrogen oxides removal process.

1.1 Literature Survey

Examination of the literature on nitrate-nitrite decomposition was facilitated by the existence of several reviews (ST-026, LE-005, SC-029, GA-038). K. H. Stern was kind enough to provide a copy of the unedited manuscript (ST-026) of his forthcoming NBS publication, "High Temperature Properties and Decomposition of Inorganic Salts. Part 3. Nitrites and Nitrates." This review covered the literature on anhydrous salts published up to 1964 and some later publications. Chemical Abstracts was used to search the literature for pertinent information published after 1964. The review by Gastwirt and Johnson (GA-038) was not obtained in time to be evaluated. The dissertations of Lee (LE-005) and Schneller (SC-029) contained detailed reviews for a limited number of compounds.

Some of the references treated in the reviews were further consulted for more details. Many references not discussed by the reviewers were also consulted. In some cases, only the abstract of a reference was consulted. In those cases, the volume and number from Chemical Abstracts is given in the bibliography. Details were gathered concerning experimental methods, phase transitions, decomposition behavior and products, and proposed reactions. These details were tabulated in a consistent form for each metal nitrate and nitrite. The tabulated data are presented and discussed in Section 2.0.

1.2 Significance of the Nitrate-Nitrite Thermal Decomposition Process

Thermal decomposition is being considered as a possible method of regeneration for the products of a nitrogen oxides removal process. One way of evaluating nitrate decomposition as a regeneration process is to examine the energy requirements, i.e., to compare the relative magnitudes of the free energy changes involved when different metal nitrates undergo decomposition in a specified temperature range. This evaluation method was applied in the thermodynamic screening of sulfate decomposition processes for regeneration of metal oxide SO_2 sorbents (LO-017).

In the case of nitrate decomposition, thermodynamic screening based on simple well-defined decomposition reactions is difficult to apply. A series of complex, interdependent reactions take place during decomposition. Gaseous decomposition products react with each other in a manner that can be represented by the series of reactions given in (1-1) through (1-5)

$$NO + NO_2 \rightleftarrows N_2O_3 \qquad (1\text{-}1)$$
$$2NO_2 \rightleftarrows N_2O_4 \qquad (1\text{-}2)$$
$$N_2O_3 + H_2O \rightleftarrows 2HNO_2 \qquad (1\text{-}3)$$
$$N_2O_4 + H_2O \rightleftarrows HNO_2 + HNO_3 \qquad (1\text{-}4)$$
$$NO + \tfrac{1}{2}O_2 \rightleftarrows NO_2 \qquad (1\text{-}5)$$

Lee reported (LE-005) that Cho and Johnson (CH-035) also found nitrous oxide, N_2O, among the reaction products of lithium nitrate decomposition. The product, found using mass spectroscopy, was not reported by many other authors as a decomposition product. As pointed out by Lee (LE-005), (1) it probably wasn't noticed since it is only produced in small amounts, and (2) if alkaline absorption were used as the method of analysis, N_2O would show up as NO.

A computer program has been written (see Technical Note 200-007-03) to calculate the existing number of moles of each of the species appearing in the above equations under given conditions of temperature, pressure and total chemical NO and NO_2. This program does not consider the effects of reaction (1-5). The program was written to describe gas phase conditions in aqueous scrubbers where the residence time and temperature limits are such that the reaction in (1-5) is kinetically limited. This may not be the case at the higher temperatures encountered in thermal decomposition.

Gaseous decomposition products also react with the product oxides and nitrites in secondary reactions that may be partially inhibited by removing gaseous products in a flowing gas stream. However, the secondary reactions may also occur in the melt where the gaseous products exist as bubbles before they are evolved. Therefore removal of the product gases after they have already left the melt would not entirely inhibit side reactions.

The complications discussed above prohibit the formulation of a simple, realistic, generalized decomposition reaction for which a free energy change may be calculated that gives a meaningful description of the decomposition process. With careful evaluation of assumptions, valuable calculations may be made. Stern (ST-026) and Kelley (KE-021) have made equilibrium calculations based on simplified reactions and involving some assumptions about activities in the melt. The only gas phase reaction considered was (1-5). Their calculations were limited, however, by the lack of both high temperature heat capacity data and standard state thermodynamic properties for some of the nitrates and most of the nitrites. The reported thermodynamic properties of the anhydrous and hydrated nitrates and nitrites and the gaseous species have been collected and tabulated in a

data base and the missing properties including high temperature heat capacities have been estimated for the anhydrous salts (see Technical Note 200-007-04). Therefore, the possibility now exists of calculating equilibrium constants (free energies) for any reaction involving oxides, nitrates, nitrites and the gaseous species of interest. The problem of formulating a representative reaction still remains.

2.0 TABULATED DATA

The details collected from the literature concerning nitrate-nitrite behavior are summarized in Table I. Temperatures and enthalpies of crystalline phase transitions and melting points are listed under the column heading "Transitions." Experimental details of decomposition experiments, temperatures of significance in the decomposition process, products identified and reactions proposed are listed under the column heading "Decomposition." References are given in the Bibliography in Section 4.0. Table I is included at the end of Section 3.

The temperatures of significance listed in the Decomposition Section should be considered carefully. "Decomposition temperature" is not a meaningful description unless the author has specified what he has observed as evidence of decomposition. One accepted definition is "that temperature at which the partial pressure of the gaseous decomposition products reached 1 atmosphere." It is doubtful that any of the temperatures listed in Table I refer to the decomposition temperature so defined. Many are given as results of TGA studies and refer to the temperature at which weight loss corresponding to nitrogen oxides evolution began. Others simply refer to the temperature at which some visible evidence of decomposition such as bubbling or evolution of either O_2 or brown NO_2 fumes was apparent.

Others refer to the temperature at which the decomposition rate was the greatest. Another accepted definition (KU-005) is the temperature at which there is a sharp break in conductance through a capillary tube containing the salt. Since molten nitrates or nitrate-nitrite mixtures find some practical applications, many studies have been conducted to determine (1) the lowest temperature at which nitrate ion begins to break down in the melt and (2) the range of temperatures over which decomposition occurs but is still slow enough that the melt can be used in the process of interest. Kust and Burke (KU-005, KU-012) have observed nitrite ion in pure $NaNO_3$ - KNO_3 eutectic melts as low as 295°C, indicating that some decomposition has already taken place. This type of information is valuable for determining the onset of decomposition but not the temperature required for rapid reaction rates.

3.0 DISCUSSION

This section contains some generalizations that can be made after examining the data summarized in Table I. It also gives some explanations proposed by various authors for the variations in thermal stabilities of nitrates and nitrites. Some proposed mechanisms and the possible paths for nitrite-nitrate decomposition are also presented.

The decomposition of metallic salts of oxyanions has been described by Stern (ST-025) as decomposition of the oxyanion accompanied by change of the metal from occupying a nitrate to occupying an oxide lattice. Such reasoning would lead to the prediction that all nitrates (sulfates, carbonates, etc.) decompose around the temperature at which the nitrate (sulfate, carbonate, etc.) ion became unstable. Variations in thermal stability of metal nitrates must therefore be explained by some property of the metal ion. One such property is the cation polarizing power, or the ability to distort the anion which is determined by the electronic configuration of the cation. Several authors (SH-017, LA-011, TK-001, AL-006, BO-008) have noticed that thermal stability increases with the decrease in polarizing power or electronegativity from lithium to cesium or beryllium to barium. The polarizing power is described quantitatively by the term e/r^2 where e is the electron charge and r the ionic radius. Obviously, as the ionic radius increases from lithium to cesium and beryllium to barium the polarizing power decreases and the ionic character increases.

Other indications of thermal stability have been discussed. Tkach (TK-001) pointed out that melting points and decomposition temperatures usually increase with heat of formation. Stern (ST-025) discussed the usefulness of free energy functions for describing thermal stability. He developed a correlation for the heat of the decomposition reaction forming N_2O_5 and metal oxide as a function of $r^{\frac{1}{2}}/Z^*$. Z^* is the effective nuclear charge felt by the electron in a bond and r is the covalent metallic radius. Stern (ST-026) and Bordyushkova, et al. (BO-008) pointed out the difference in stability and behavior of ionic and covalent nitrates. Stern's generalizations were as follows:

- Ionic nitrates, in which the nitrate ion is a distinct entity (not distorted or deformed) such as it exists in aqueous solutions, melt to form stable liquids.
- Some decomposition of the melt from nitrate to nitrite occurs, and the nitrites and nitrates are stable within overlapping temperature ranges. Therefore the decomposition path is complicated.

- Ionic nitrates have higher decomposition temperatures than covalent nitrates.

- Covalent nitrates, which exhibit some metal-oxygen bonding, often do not form stable melts. In some cases they even sublime.

The first step in nitrate decompositions is then generally recognized as formation of nitrite which may or may not be stable at the nitrate decomposition temperature. The nitrite may then decompose to the oxide. The nitrite decomposition path is similarly complicated. Nitrites usually decompose to the oxide, which again can be converted to nitrate by the reaction products. Some of the nitrite can also be oxidized to nitrate by the decomposition products. Usually the nitrates are more stable than the nitrites so that complete decomposition to the oxide cannot occur until some temperature above the range of nitrate stability has been reached. Other reported decomposition intermediates besides nitrites and oxides are the basic oxynitrates.

The generalizations discussed above are illustrated in Table II, which gives in periodic arrangement some significant temperatures (melting, slow and rapid decomposition, and oxide formation) taken from Table I and a description of ionic or covalent character taken from Stern (ST-026). Some of the variations in temperature are a result of the experimental methods such as heating rate for different TGA experiments. From Table II it can be seen at a glance that thermal stability increases from lithium to cesium and beryllium to barium. It is also evident that the ionic alkali metal nitrates are stable above their melting points. In fact, decomposition is even slow from 100 to 300° above the melting points where the melts are still considered thermally stable for practical use (BO-008). The temperatures for oxide formation were not found for the alkali metal nitrates. Gordon and Campbell (GO-014) reported that in general decomposition was still occurring around 900°C. The same trend is not as pronounced for the alkaline earth nitrates. Decomposition occurs before or in the same temperature range as the melting point. As a result there may be wide variations in reported melting points such as the case for strontium nitrate. One author was able to completely decompose calcium nitrate below its melting point with slow heating, while another was not capable of carrying out decomposition rate measurements at higher temperatures because of spattering of the melt.

The temperatures summarized in Table II are for both hydrates and anhydrous nitrates. Tkach (TK-001) reported the anhydrous salts given slower decomposition rates than the hydrates and Gordon and Campbell (GO-014) commented that hydrates decompose at lower temperatures than anhydrous nitrates. These claims do not seem to be substantiated by the data in Table I. Gordon and Campbell may have been referring to the fact that metal nitrates such as those of Zn, Cd and Hg, which exist as the hydrates, are generally less thermally stable than the anhydrous alkali metal and alkaline earth nitrates.

TABLE 11

TEMPERATURES OF SIGNIFICANCE IN NITRATE THERMAL DECOMPOSITION

* Ionic Bonding
** Covalent Bonding

																H	He
Li* m. 253 Slow 393 Meas. 383-420 High >457	Be** m. ? High >125 TGA Range 175-200 Oxide 460											B	C	N	O	F	Ne
Na* m. 306-308 Slow 600	Mg* m. Slow 327 Oxide 430-455											Al** Rate Measure-able 160-80 Oxide: Al_2O_3 390-460	Si	P	S	Cl	Ar
K* m. 336-7 Slow 530-65	Ca* m. 561 Slow 475-575 Oxide 665	Sc	Ti** m. 58 No dec <58	V	Cr** Fast 60-100 Oxide: Cr_2O_5 200 Cr_2O_3 665	Mn** Slow 160 Fast 230 Oxide: MnO_2 280	Fe** m. 35-100 Slow Room Temp. Oxide: Fe_2O_3 405-50	Co* Slow 100 Fast 170-270 Oxide: Co_3O_4 280-315	Ni** m. 50-57 Slow 105-260 Fast >260 Oxide: NiO 300-500	Cu*** m. 255 Slow 227 Rapid 300 Oxide: CuO 300-50	Zn** Slow 100-260 Rapid 330 Oxide: ZnO 340-470	Ga Oxide: GaO 200	Ge	As	Se	Br	Kr
Rb* m. 310 Slow 312-600	Sr* m. 570-645 Slow 480 Oxide 645-680	Y	Zr** Oxide: ZrO_2 575	Nb	Mo	Tc	Ru	Rh	Pd**	Ag* m. 210-21 Slow 440 Fast 260-30 Metal 600	Cd** Rapid >300 Oxide: CdO 635-54	In** Slow >90	Sn** m. 91 Slow 98	Sb	Te	I	Xe
Cs* m. 405-15 Slow 555	Ba** m. 588-95 Slow 560-64 Rapid 692	La**	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg**	Tl* m. 205-10 Slow 265	Pb* Slow 265 Rapid > 370 Oxide: PbO_2 575	Bi** Slow 90 Fast 100-25 Oxide: Bi_2O_3 560-60	Po	At	Rn
Fr	Ra	Ac															

TABLE I - DECOMPOSITION BEHAVIOR OF ANHYDROUS AND HYDRATED NITRITES AND NITRATES

	TRANSITIONS				DECOMPOSITION					
COMPOUND	T(°C)	Type	ΔH(Kcal/mole)	Ref.	T(°C)	Method/Comments	Products	Reactions	Ref.	DISCUSSION
1. $LiNO_2$	220	S-L		ST-026	300 350 >350	Stable Slow decomposition. More rapid decomposition.	NO, NO_2	$2LiNO_2 \rightleftarrows Li_2O + NO + NO_2$ (1)	ST-026	Stern (ST-026) reports the gaseous products oxidize the nitrite to nitrate if they are not removed.
	96 226	S-S S-L		PR-003		A thin 2.0 cm layer of molten nitrite was contained in a platinum dish under a flowing argon atmosphere in a muffle furnace. Temperature was constant ± 1°C. Experiments were done at 250, 300, 350, and 450°. Compositions of the melt and gas phase were determined after 0, 1, 2, 3, 4, 5 and 6 hours.	At 250 to 350: O_2, N_2, N_2O, NO, $LiNO_3$, Li_2O. NO_2 given off above 450.	$2LiNO_2 \rightleftarrows Li_2O + N_2O_3$ (2) $N_2O_3 \rightleftarrows NO + NO_2$ (3) Reactions involving products: $LiNO_2 + N_2O_3 \rightleftarrows LiNO_3 + 2NO$ (4) $2LiNO_2 + N_2O_3 \rightleftarrows 2LiNO_3 + N_2O$ (5) $Li_2O + 2NO_2 \rightleftarrows LiNO_2 + LiNO_3$ (6) $2LiNO_2 + 2NO \rightleftarrows 2LiNO_3 + N_2$ (7) $2LiNO_3 \rightleftarrows 2LiNO_2 + O_2$ (8)	LE-005	The reactions were found to be mainly homogeneous (in the melt) rather than to involve gaseous nitrogen oxides. N_2O_3 and NO_2 concentrations in the molten phase are very small; both are consumed in other reactions in the melt as soon as they were formed (reactions 4, 5, and 6). Reaction (7) was found to be strongly temperature dependent. The wide range of proportions of N_2 and NO found at different temperatures is attributed to the temperature dependence of this essentially irreversible reaction. The sequence of reactions is in the order 4, 5, 7, and 8. After a certain period, (7) becomes rate controlling. The rate at which a steady decomposition was obtained was found to depend on the solubility of gases in the melt. The mechanism for this decomposition appears to depend on temperature and melt composition. The stoichiometries are different at 250, 300, and 350. The reaction at 450 is the only one for which NO_2 could be detected in the gaseous products. This agreed with the reports by Peneloux (PE-015) that a rapid, high temperature decomposition produced NO_2 while a slow, low temperature decomposition produced NO. The solubilities of NO and NO_2 in the melt can (cont.)
					160	NO was first detected at 160°. Kinetic runs were not possible at 450° since the reaction vessel overflowed.				

	TRANSITIONS				DECOMPOSITION					
COMPOUND	T(°C)	Type	ΔH(Kcal/mole)	Ref.	T(°C)	Method/Comments	Products	Reactions	Ref.	DISCUSSION
1. $LiNO_2$ (cont.)										probably account for part of these results. The decomposition rate was considerably faster at 450, and NO_2 was detected in the gas. The decomposition is still slow at 350.
2. $LiNO_3$	120 170 230 253	S-S S-S S-S S-L	 6.04	SC-012 PR-003 ST-026 SC-012 BO-008	293 383-420 >457	Decomposition begins slowly at about 40° above the melting point. Measurable O_2 pressures achieved in this range. Rate is appreciable only in this range.	O_2	$LiNO_3 \rightleftarrows LiNO_2 + \frac{1}{2}O_2$ (9a)	ST-026	Stern reports oxides of nitrogen can also be formed if container material is not inert. Nitrite product dissolves in melted nitrate.
					450,500	Nitrate still stable.	O_2, N_2O	$LiNO_3 \rightleftarrows LiNO_2 + \frac{1}{2}O_2$ (9a) $LiNO_3 + LiNO_2 \rightleftarrows Li_2O + 2NO_2$ (9b)	CH-035	The rate constants for (9a) were measured at 450 and 500°C. Nitrous oxide (N_2O) was detected in the gaseous products using mass spectrometry.
3. $LiNO_3 \cdot 3H_2O$	29.9	S-L	8.33	NE-004						
4. $NaNO_2$	162 281 166 283 161	S-S S-L S-S S-L S-S	.299 2.48 .285	AD-002 ST-026 PR-003 PR-003 NO-005	>330	Nitrite unstable above 330.	N_2O_3, NO, NO_2, Na_2O	$2NaNO_2 \rightleftarrows Na_2O + NO + NO_2$ (10)	ST-026	If the gas phase is continually removed, this is the only reaction that occurs.
					330-380	Nitrate is formed.	N_2, NO, $NaNO_3$	$2NaNO_2 + 2NO \rightleftarrows 2NaNO_3 + N_2$ (11) $Na_2O + 2NO_2 \rightleftarrows NaNO_2 + NaNO_3$ (12) $NaNO_2 + NO_2 \rightleftarrows NaNO_3 + NO$ (13)	ST-026	These are the reactions involving the products NO and NO_2 and the remaining nitrite. The nitrate is stable in this temperature range and N_2 is unreactive (ST-026).
					600-750	Nitrate begins to decompose to nitrite.	O_2	$NaNO_3 \rightleftarrows NaNO_2 + \frac{1}{2}O_2$ (14)	ST-026	The activation energy for this reaction has been reported as 44.7 and 40.3 kcal.
					600-750	Nitrite decomposes to the oxide.	N_2, O_2	$2NaNO_2 \rightleftarrows Na_2O + N_2 + 3/2\ O_2$ (15)	ST-026	The activation energy for this reaction has been reported as 42.8 kcal. Decomposition of NO and NO_2 to the elements has been considered kinetically limited. (cont.)

	TRANSITIONS				DECOMPOSITION					
COMPOUND	T°C)	Type	ΔH(kcal/mole)	Ref.	T(°C)	Method/Comments	Products	Reactions	Ref.	DISCUSSION
4. $NaNO_2$ (cont.)										A mechanism of N_2 production has therefore been suggested which involves the formation of a super oxide which decomposes to Na_2O and O_2
						Study of the action of NO on Na_2O.	N_2, N_2O, $NaNO_2$	$Na_2O + 3NO \rightleftarrows 2NaNO_2 + \frac{1}{2}N_2$ (16) $Na_2O + 4NO \rightleftarrows 2NaNO_2 + N_2O$ (17)	CH-036	In order to account for the formation of nitrous oxide and N_2, reactions (16) and (17) were proposed.
						The $NaNO_2$-NO_2 system was studied.	NO, $NaNO_3$	$NaNO_2 + NO_2 \rightarrow NaNO_3 + NO$ (18)	OZ-006	At temperatures above 250, the rate of the reaction $NO_2 \rightarrow NO + \frac{1}{2}O_2$ becomes appreciable. NO production and NO_2 consumption affect nitrite oxidation. The reaction proceeds to the left rather than the right.
					150	No reaction.				
					200	10% conversion of $NaNO_2$ to $NaNO_3$.				
					250	Maximum extent of reaction.				
					> 250	Reaction (as written) diminishes.				
5. $NaNO_3$	160	S-S		SC-012	500	Liquid $NaNO_3$ still stable.	$NaNO_2$	$NaNO_{3(l)} \rightleftarrows NaNO_{2(l)} + \frac{1}{2}O_2$ (19)	ST-026	The liquid nitrates and nitrites are reported to be completely miscible and are reported to form a "virtually ideal" solution (ST-026). The equilibrium constants for $2NaNO_{3(s)} \rightarrow Na_2O_{(s)} + 2NO_{2(g)} + \frac{1}{2}O_{2(g)}$ to 700°K and $NaNO_{3(l)} \rightarrow NaNO_{2(l)} + \frac{1}{2}O_2$ from 800 to 1000°K have been calculated (ST-026).
	275	S-S	1.12	FE-003	600	Slow decomposition of melt.				
	306	S-L	3.70	ST-026	600-750	Pseudo equilibrium between air and melt containing $NaNO_3$ and $NaNO_2$.				
	308	S-L		BO-008						
					510	Decomposition begins as evidenced by appearance of .05% nitrite in the melt.		Same	BO-008	
6. KNO_2	47	S-S	0.199	PR-003 AD-002	410-460	Noticeable decomposition. Inert atmosphere with gaseous products removed.	NO_2, NO, K_2O	$2KNO_2 \rightleftarrows K_2O + NO_2 + NO$ (20)	ST-026	Gaseous products react with KNO_2 and K_2O if they are not removed.
	437	S-L		PR-003						
	440	S-L		ST-026						
					(cont.)	(cont.)	(cont.)	(cont.)	(cont.)	(cont.)

	TRANSITIONS				DECOMPOSITION					
COMPOUND	T(°C)	Type	ΔH(kcal/mole)	Ref.	T(°C)	Method/Comments	Products	Reactions	Ref.	DISCUSSION
6. KNO_2 (cont.)					410-460	In air, without gaseous product removal, nitrate is still stable.	N_2, NO, KNO_3	$2KNO_2 + 2NO \rightleftarrows 2KNO_3 + N_2$ (21) $K_2O + 2NO_2 \rightleftarrows KNO_2 + KNO_3$ (22) $KNO_2 + NO_2 \rightleftarrows KNO_3 + NO$ (23)	ST-026	KNO_3 is stable in this temperature range.
					550-750	In oxygen atmosphere nitrate begins to decompose.		$KNO_2 + \frac{1}{2}O_2 \rightleftarrows KNO_3$ (24)	ST-026	Up to 600 the KNO_3 remains stable. Between 600 and 750 the reaction is in equilibrium since the KNO_3 is unstable.
					>800	Nitrite decomposes to oxide.	K_2O	$KNO_2 \rightarrow K_2O + \frac{1}{2}N_2 + \frac{1}{2}O_2$ (25)	ST-026	
						KNO_2 in NO_2 atmosphere.	NO, KNO_3	$KNO_2 + NO_2 \rightleftarrows KNO_3 + NO$ (23)	OZ-006	The reaction is reversible with the maximum KNO_3 formation at 200. Apparently it is difficult to establish equilibrium since the rate of the reaction $NO_2 \rightleftarrows NO + \frac{1}{2}O_2$ becomes appreciable. Above 200, then, the amount of KNO_3 produced decreases.
					130	No reaction as written.				
					140	Considerable reaction rate.				
					200	Reaction rate is at a maximum.				
7. KNO_3	127.9 334.3	S-S S-L	1.22 2.30	YA-004	530	Melt is stable in air to this temperature.	KNO_2	$KNO_{3(l)} \rightleftarrows KNO_{2(l)} + \frac{1}{2}O_2$ (26)	ST-026	Both the kinetics and equilibrium of this reaction have been studied. The activation energy has been measured and reported to be 65.6 kcal/mole. One author reported that equilibrium was established between 650 and 750 under 1 atm oxygen. The measured equilibrium constant for the range 550 to 750 was
	113 123 128 334	S-S S-S S-S S-L	.56 .72 1.3 2.3	ST-026	650	Decomposition begins in air.				
									$\log K = \frac{-115\pm5\ KJ/mole}{2.303\ RT} + \frac{102\pm5}{2.303\ R}$	The equilibrium constant for the reaction $KNO_3 \rightarrow K_2O + 2NO_2 + \frac{1}{2}O_2$ was calculated from 298 to 1000°K by Stern (ST-026).
					530	Decomposition of the nitrate melt begins as indicated by .05% nitrite in the melt.	KNO_2	Same	BO-008	

	TRANSITIONS				DECOMPOSITION					
COMPOUND	T(°C)	Type	ΔH(kcal/mole)	Ref.	T(°C)	Method/Comments	Products	Reactions	Ref.	DISCUSSION
8. $RbNO_2$	422	S-L		PR-003	450	Stable up to this temperature. Reaction proceeds as written if the gaseous products are removed.	Rb_2O, NO, NO_2	$2RbNO_2 \rightleftarrows Rb_2O + NO + NO_2$ (27)	ST-026	If the gaseous products are not removed, the nitrite can be oxidized to nitrate. The nitrate will be stable over a particular temperature range. The behavior and reactions resemble those of the other alkali metal nitrites.
9. $RbNO_3$	160 215 281	S-S S-S S-S	0.93 0.77 0.23	ST-026	600	The salt begins to loose weight above this temperature.	$RbNO_2$	$RbNO_{3(l)} \rightleftarrows RbNO_{2(l)} + \frac{1}{2} O_2$ (28)	ST-026	The behavior should resemble that of other alkali metal nitrates.
	158 222 286	S-S S-S S-S		NY-001	512	Decomposition temperature taken as that at which .05% nitrite could be detected in the nitrate melt.	$RbNO_2$	(Same)	BO-008	Alkali metal nitrates melts are still fairly stable at temperatures even 200° above their melting points. At higher temperatures decomposition becomes more rapid.
	310	S-L	1.11	ST-026						
10. $CsNO_2$	401	S-L		PR-003	450	The salt is stable up to this temperature.	Cs_2O, NO, NO_2	$2CsNO_2 \rightleftarrows Cs_2O + NO + NO_2$ (29)	ST-026	See Discussion for $RbNO_2$ (No. 8).
	406	S-L		ST-026						
11. $CsNO_3$	151.5	S-S	0.893	MU-012	555	Decomposition temperature taken as that at which .05% nitrite could be detected in the melt.	$CsNO_2$	$CsNO_{3(l)} \rightleftarrows CsNO_{2(l)} + \frac{1}{2}O_2$ (30)	BO-008	See Discussion for $RbNO_3$ (No. 9).
	414	S-L		BO-008						
	405.5	S-L	3.37	MU-012						
12. $CsNO_3 \cdot 4H_2O$	42.7	S-L		RO-007						
13. $Be(NO_2)_2$										No evidence was found in the literature for the existence of this compound.
14. $Be(NO_3)_2$					125	Decomposition is rapid above this temperature.	$Be_4O(NO_3)_6$, NO_2		ST-026	The nitrate is a hygroscopic solid.
					(cont.)	(cont.)	(cont.)	(cont.)	(cont.)	(cont.)

	TRANSITIONS				DECOMPOSITION					
COMPOUND	T(°C)	Type	ΔH(kcal/mole)	Ref.	T(°C)	Method/Comments	Products	Reactions	Ref.	DISCUSSION
14. $Be(NO_3)_2$ (cont.)					175-200	This temperature range was established for decomposition from the thermogram recorded at a heating rate of 6-9°/min.			SH-017	It was difficult to prepare a crystalline nitrate. Usually a viscous mass was obtained This is the least stable of the alkaline earth nitrates.
15. $Be(NO_3)_2 \cdot 4H_2O$						The TGA experiments were carried out in a stream of air. Gaseous products were not analyzed			WE-021	There was no evidence (no breaks in the thermogram) for formation of the anhydrous nitrate.
					55	Salt began to loose water of hydration.				
					55-205	Maximum rate of weight loss.				
					460	No further weight loss. Oxide formed at this temperature.	BeO			
16. $Mg(NO_2)_2$						Decomposition of the nitrate in NO was studied. The nitrite was produced as a product.	Not described.	$Mg(NO_3)_2 + 2NO \rightleftarrows Mg(NO_2)_2 + 2NO_2$ (31)	ST-026	The existence of the anhydrous nitrite is uncertain. It appeared as an intermediate in the decomposition of the nitrate in NO.
					107	Nitrite product decomposes.				
17. $Mg(NO_2)_2 \cdot 2H_2O$						Method not described.	NO, NO_2, N_2	$Mg(NO_2)_2 \rightleftarrows MgO + N_2O_3$ (32a) $N_2O_3 \rightleftarrows NO + NO_2$ (32b) $Mg(NO_2)_2 + 2NO_2 \rightleftarrows Mg(NO_3)_2 + 2NO$ (31) $2MgO + 4NO_2 \rightleftarrows Mg(NO_2)_2 + Mg(NO_3)_2$ (33) $Mg(NO_2)_2 + 2NO \rightleftarrows Mg(NO_3)_2 + N_2$ (34)	LE-005	Lee (LE-005) stated that the 1905 investigations of Ray and Ganguli (complete reference not given in LE-005) indicated the nitrite decomposes at a low temperature. Lee also discussed the work of Oza and Dipali (OZ-009) carried out at 110°C. The overall stoichiometry was found by both to be $3Mg(NO_2)_2 \rightleftarrows 2MgO + Mg(NO_3)_2 + 4NO$. Apparently temperatures reached were never high enough so that decomposition of the nitrate could occur. It was concluded that the extent of reaction (34) was very slight since only small amounts of N_2 were found

	TRANSITIONS				DECOMPOSITION					
COMPOUND	T(°C)	Type	ΔH(kcal/mole)	Ref.	T(°C)	Method/Comments	Products	Reactions	Ref.	DISCUSSION
18. $Mg(NO_3)_2$					327	The solid is reported to be stable up to this temperature. The melt is reported to be unstable, but no melting point was given.		Not given.	ST-026	Stern reports that the stability depends on the gas phase. Decomposition may occur at temperatures lower than 327. Stern calculated equilibrium pressures for: $Mg(NO_3)_2 \rightleftarrows MgO + 2NO_2 + \frac{1}{2}O_2$ (35) The calculations indicated decomposition would be complete between 500 and 600°K (327°C)
					127	Decomposition occurs at this temperature if nitric oxide is present.				
19. $Mg(NO_2)_2 \cdot 2H_2O$	130	S-L		RO-007						
20. $Mg(NO_3)_2 \cdot 6H_2O$	90	S-L	9.8	LA-008	60	Begins losing water of hydration.	Final Product: MgO		WE-021 BE-036	Three thermogravimetric studies have been reported for the hexahydrate (BE-036, SH-018, WE-021). The temperatures reported for heat effects are in fair agreement. No reactions were proposed however and neither the gaseous products nor the intermediates were analyzed. The results agree fairly well with Stern's estimate of the range of stability for the nitrate
					80-90	Endothermal effect (SH-018).				
					85-90	Endothermal effect (BE-036).				
					125-180	Unidentified thermal effect (SH-018).				
					145-150	Endothermal effect (BE-036).				
					230	Formation $Mg(NO_3)_2 \cdot 2H_2O$ (BE-036).				
					240	Formation $Mg(NO_3)_2 \cdot H_2O$ (WE-021).				
					310	Formation $Mg(NO_3)_2$ (WE-021).				
					370	Formation $Mg(NO_3)_2$ (BE-036).				
					430	Formation MgO (BE-036).				
					455	Formation MgO (WE-021).				
								$Mg(NO_3)_2 \rightleftarrows MgO + 2NO_2 + \frac{1}{2}O_2$ (35)	KE-021	Kelley (KE-021) stated the hexahydrate is the form that crystallizes from water at ordinary temperatures. He calculated the free energy (cont.)

	TRANSITIONS				DECOMPOSITION					
COMPOUND	T(°C)	Type	ΔH(kcal/mole)	Ref.	T(°C)	Method/Comments	Products	Reactions	Ref.	DISCUSSION
20. $Mg(NO_3)_2 \cdot 6H_2O$ (cont.)										of the dehydration reaction at 300, 350, 400, 450 and 500°K. The data indicated that dehydration would be complete near 450°K (172°C). Free energy calculations for (35) indicated a decomposition pressure of 1 atm would be reached at 288°C.
21. $Ca(NO_3)_2$	266	S-S		ST-026	267-315	Decomposition pressures were measureable in this temperature range.	Mainly NO	$Ca(NO_3)_2 \rightleftarrows CaO + NO + NO_2$ (36) $Ca(NO_2)_2 + 2NO_2 \rightleftarrows Ca(NO_3)_2 + 2NO$ (37)	ST-026	Stern reports (36) and (37) were the reactions for which decomposition pressures were measured. Reaction (36) should probably be written $Ca(NO_3)_2 \rightleftarrows CaO + N_2O_3$ (36) $N_2O_3 \rightleftarrows NO + NO_2$ (32b) However, the temperatures at which the decomposition was studied were below the reported melting point. This fact is inconsistent with the accepted idea that nitrate-nitrite melts are relatively stable from 50 to 100° above their melting point. The reported transition points were taken from heating curves and the nature of the phases was not described (ST-026).
	380	S-S		ST-026						
	392	S-L		ST-026						
					370-480	Reaction (38) becomes important.	NO, N_2	Same as (36) and (37), as well as $Ca(NO_2)_2 + 2NO \rightleftarrows Ca(NO_3)_2 + N_2$ (38)	ST-026 LE-005	Stern and Lee both discussed the 1953 work of Oza and Oza. Only small amounts of N_2 were detected in agreement with the reports of early workers. This was accounted for by the explanation that at higher temperatures the reverse of (37) becomes more important and there exists less NO to react as in (38). Note that the reaction involving the oxide and NO_2, such as reaction (33) for MgO, was not proposed.
					(cont.)	(cont.)	(cont.)	(cont.)		(cont.)

	TRANSITIONS				DECOMPOSITION					
COMPOUND	T(°C)	Type	ΔH(kcal/mole)	Ref.	T(°C)	Method/Comments	Products	Reactions	Ref.	DISCUSSION
21. $Ca(NO_2)_2$ (cont.)					420-450	The decomposition in this temperature range was studied in argon, air, and under vacuum. Reaction (39) becomes important in this range.	NO, N_2	$4Ca(NO_2)_2 \rightleftarrows 2Ca(NO_3)_2 + 2CaO + 2NO + N_2$ (39)	ST-026 LE-005	Stern and Lee also both commented on the rate studies of Protsenko and Bordyushkova published in 1965. The overall stoichiometry in argon was given by (39). The nitrate is still relatively stable in the temperature range studied. The decomposition rates in air and vacuum were greater than in argon. Rate constants and an activation energy were calculated for (39).
					Temperatures above the decomposition temperature of the nitrate.		O_2, N_2, NO, NO_2	$2CaO + 4NO_2 \rightleftarrows Ca(NO_3)_2 + Ca(NO_2)_2$ (40) $Ca(NO_3)_2 \rightleftarrows Ca(NO_2)_2 + O_2$ (41)	LE-005	The relative amounts of the products formed in this range depend on the temperature and the duration of decomposition and the amount of nitrite undergoing decomposition (LE-005). Lee suggests that ultimately the nitrite decomposition rate is dependent on the rate of reactions involving $Ca(NO_3)_2$ and CaO in the melt.
22. $Ca(NO_2)_2 \cdot H_2O$						The nitrite, mixed with charcoal, was evacuated and heated in stages to 400°. The gaseous products were analyzed as well as the solid residue.	Mostly NO. Some N_2 and N_2O. CO_2 only at 280. $CaCO_3$; CaO.	$Ca(NO_2)_2 \rightleftarrows CaO + NO + NO_2$ (36) $C + N_2O_3 \rightleftarrows CO_2 + N_2O$ (42) $C + 2NO_2 \rightleftarrows CO_2 + 2NO$ (43) $C + 2NO \rightleftarrows CO_2 + N_2$ (44) $CaO + CO_2 \rightleftarrows CaCO_3$ (45) $2CaO + 4NO_2 \rightleftarrows Ca(NO_3)_2 + Ca(NO_2)_2$ (40)	OZ-003	Oza stated that earlier workers have noticed nitrite decomposition beginning at 330 and 360. His work showed that the decomposition begins at 280 when CO_2 was first evolved. It is probably slow at that temperature and could go unnoticed if the nitrogen oxides reacted in the melt. In the presence of charcoal, however, the product nitrogen oxides would rather react to form CO_2 than react with CaO or $Ca(NO_2)_2$. In fact, nitrate was found in the residue only in 4 hour experiments at 410° when smaller amounts of charcoal were added. A further result is that the nitrate can be only partially dehydrated without decomposition.
					80	Dehydration (3/4 the water).				
					280	CO_2 first evolved. Also NO and N_2. N_2O analysis not performed. Nitrite decomposition began at this temperature.				
					350	NO, N_2 evolved. No N_2O present.				
					400	NO and N_2 evolved in greater quantities.				
					(cont.)	(cont.)	(cont.)	(cont.)		(cont.)

	TRANSITIONS				DECOMPOSITION					
COMPOUND	T(°C)	Type	ΔH(kcal/mole)	Ref.	T(°C)	Method/Comments	Products	Reactions	Ref.	DISCUSSION
22. $Ca(NO_2)_2 \cdot H_2O$ (cont.)					0.2	A mixture of NO and NO_2 was passed slowly over CaO for 1-2 hours. The gas phase was analyzed only for total nitrogen oxides. The temperature was low to prevent decomposition of nitrites, if formed.	$Ca(NO_3)_2$	$CaO + 2NO_2 + \frac{1}{2}O_2 \rightarrow Ca(NO_3)_2$ (46)	OZ-004	This experiment was performed to test the validity of (36). $Ca(NO_2)_2 \rightleftarrows CaO + NO + NO_2$ (36) The conclusion was that, since only nitrates were formed by sorption, (36) could not be the correct way to describe the first step in nitrite decomposition.
					360	The nitrite was decomposed at this temperature for periods of 1, 2, 3, and 4 hours The gaseous products were removed.	Mostly NO, Some NO_2. Very little N_2. No analysis made for N_2O.		OZ-004	The residue was analyzed after 1, 2, 3, and 4 hours. Nitrate production decreased with time while nitrite was continually used up and oxide production increased. Since the gaseous products were continually removed, there must have been some reaction in the melt to produce nitrate. Oza claimed reaction of CaO and NO_2 according to (46). The oxidation of calcium nitrite is also a possibility, either by (37) or (38).
					500	Nitrite decomposition was studied at this temperature under the following conditions. a) Gaseous products not removed. b) Oxygen atmosphere. c) Vacuum. In each experiment, the residue was analyzed after 10 minutes.	$Ca(NO_3)_2$, CaO, gas phase analyses not complete.		OZ-004	The relative amounts of $Ca(NO_3)_2$ and CaO formed under different conditions were studied as well as the rate of nitrate decomposition. The rate was greater in vacuum than in O_2 or when the gaseous products were not removed. Naturally the proportion of nitrate formed per mole of decomposed nitrite was greatest in the O_2 experiments since NO could be oxidized to NO_2. The rate of decomposition also increased when CaO was added to the nitrite to be decomposed.

	TRANSITIONS				DECOMPOSITION					
COMPOUND'	T(°C)	Type	ΔH(kcal/mole)	Ref.	T(°C)	Method/Comments	Products	Reactions	Ref.	DISCUSSION
23. $Ca(NO_3)_2$	561	S-L	5.09	LA-008		No experimental measurements performed.		$Ca(NO_3)_2 \rightleftarrows CaO + 2NO_2 + \frac{1}{2}O_2$ (47)	ST-026	Stern (ST-026), finding no data published prior to 1964 on decomposition of the anhydrous salt, calculated thermodynamic data for reaction (47) from 25 to 527°C. A dissociation pressure of 0.6 atm was calculated for 527°C although the reported melting point is 561°.
						CaO pellets were packed into an absorption chamber and 10% NO_2 in N_2 was circulated at a rate of .19 moles/hr.		$2CaO + 4NO_2 \rightleftarrows Ca(NO_3)_2 + Ca(NO_2)_2$ (40)	AT-010	The rate of absorption of NO_2 on CaO was studied and the products were the nitrate and the nitrite. These results are in contrast to those found at 0°C by Oza for absorption of a mixture of NO and NO_2. Oza reported no nitrite formation at all.
					250-350	The rate of reaction (40) is maximum in this temperature range. $Ca(NO_2)_2$ is oxidized to $Ca(NO_3)_2$ beginning at 250°.				
					575	Lazarini and coworkers cited 575°C from an earlier publication by Addison as the temperature at which bubbles appeared in a calcium nitrate melt.			LA-011 (Addison)	
					475	Lazarini also cited this temperature from Duval's TGA measurements as the one at which decomposition began. He stated that it is commonly found that alkaline earth nitrates begin to decompose at temperatures below their melting point.			LA-011 (Duval)	
					(cont.)	$Ca(NO_3)_2$ was prepared by drying the tetrahydrate at 120 or 160°C for 24 hrs. The decomposition of the anhydrous salt was studied on a (cont.)		Not given.	LA-011 (cont.)	From the thermogram it was evident that weight loss began at 455°C. It was not possible to carry out the decomposition at the 5°C/min. heating rate because (cont.)

	TRANSITIONS				DECOMPOSITION					
COMPOUND	T(°C)	Type	ΔH(kcal/mole)	Ref.	T(°C)	Method/Comments	Products	Reactions	Ref.	DISCUSSION
23. $Ca(NO_3)_2$ (cont.)						thermobalance at a heating rate of 5°C/min. Gaseous reaction products were removed by a flowing stream of N_2.				spattering occurred. Therefore, it is not known at what temperature the residue consisted of oxide.
					455	Decomposition began at this temperature.				
						Isothermal measurements of the variation of weight loss with time were made at 440, 450, 460 and 475. Gaseous products were removed.	CaO, gaseous products not analyzed.	None given.	LA-011	From the shape of the weight loss curves obtained isothermally, a physical description of the decomposition mechanism was obtained. First the nitrate begins to decompose to a limited extent. Then it begins to melt and the weight loss curve becomes linear. Gas bubbles were observed in the melt. Finally the solid phase (CaO) crystallizes from the melt and at the same time the weight reaches a constant value. According to Lazarini's mechanism, the rate of decomposition is limited by diffusion of the gaseous decomposition products (bubbles) at the phase boundary. It is stated that the surface area is reduced by melting and then remains constant, so that a constant decomposition rate results.
						Prolonged heating and degassing at 120 and 200 were used to produce the anhydrous salt. The decomposition was studied at temperatures below the melting point (470 to <550). Gaseous products were removed only periodically. (cont.)	O_2, NO, NO_2; neither N_2, N_2O nor N_2O_4 could be detected. The condensed phase was not studied.	None given.	BO-009	The decomposition was slow at 470, but small increases in temperature caused a great increase in reaction rate. The amount of oxygen evolved was constant throughout the reaction. The production of NO went through a minimum in the middle of the reaction; at the same time, a maximum in NO_2 production occurred.

	TRANSITIONS				DECOMPOSITION					
COMPOUND	T(°C)	Type	ΔH(kcal/mole)	Ref.	T(°C)	Method/Comments	Products	Reactions	Ref.	DISCUSSION
23. $Ca(NO_3)_2$ (cont.)						Decomposition was continued by raising the temperature (still below the melting point) until no more gas evolution was noticed. The decomposition was slow, no melting or spattering occurred, and the product was in the form of well distinguished crystals.				
						The decomposition was studied by thermogravimetry at a heating rate of 6-9°/min.	Not given.	Not given.	SH-017	No comments were made in the abstract concerning the composition of the residue or the gaseous production.
					480-500	The decomposition was found to take place in this temperature range.				
						DTA was used to study $Ca(NO_3)_2$ decomposition. The heating rate was 15°C/min. Endotherms were recorded at 552, 609, and 642.	"nitrous fumes"	None given	GO-014	See discussion for $Sr(NO_3)_2$, (No. 26).
					550	Fusion				
					581	Rapid bubbling.				
					642	Rapid evolution of nitrous fumes.				
24. $Ca(NO_3)_2 \cdot nH_2O$						The following temperature ranges of stability were found for the hydrates.	Not described.	None given.	GL-008	This work was done in a study of the evaporation and crystallization of solutions containing nitrates, carbonates, and sulfates.
					26-126	Tetrahydrate				
					126-215	Trihydrate				
					215-315	Dihydrate				
					315-435	Monohydrate				
					(cont.)	(cont.)	(cont.)	(cont.)	(cont.)	(cont.)

	TRANSITIONS				DECOMPOSITION					
COMPOUND	T(°C)	Type	ΔH(kcal/mole)	Ref.	T(°C)	Method/Comments	Products	Reactions	Ref.	DISCUSSION
24. $Ca(NO_3)_2 \cdot nH_2O$ (cont.)					435	Anhydrous nitrate				
					>500	Nitrate decomposition.				
								$Ca(NO_3)_2 \rightleftarrows CaO + 2NO_2 + \frac{1}{2}O_2$ (47)	KE-021	Kelley reported the tetrahydrate crystallizes from water at ordinary temperatures. This is in agreement with Gladushko (GL-008). Kelley also states that the tetrahydrate can be dehydrated without decomposition and that the dehydration sequence involves the tetrahydrate, the trihydrate and the dihydrate with no formation of the monohydrate. These results are in contrast to those of Gladusko (GL-008) who reported the formation of the monohydrate in the range 315-435. Kelley calculated the free energy of (47) as a function of temperature up to about 600°C. He found that the decomposition pressure becomes 1 atm at 544°C if the N_2 forming reaction is neglected.
						Thermogravimetric analysis was used to study the decomposition of the tetrahydrate. The heating rate was 5°C/min. and a slow stream of air was passed through the furnace. The following temperatures of interest were noted.	CaO, gas phase not studied.	None given.	WE-021	Wendlandt's results for the range of stability of the anhydrous salt agree with those of Gladushko (GL-008). However, no evidence of monohydrate formation was found. The temperatures of formation for the tri- and dihydrates were quite easily distinguished from the heating curve. Note that Lazarini reported he was unable to carry out the decomposition at a heating rate of 5°C/min, the same as used by Wendlandt, because of spattering.
					50	Began losing water.				
					130	Formation $Ca(NO_3)_2 \cdot 3H_2O$				
					160	Formation $Ca(NO_3)_2 \cdot 2H_2O$				
					(cont.)	(cont.)				

	TRANSITIONS				DECOMPOSITION					
COMPOUND	T(°C)	Type	ΔH(kcal/mole)	Ref.	T(°C)	Method/Comments	Products	Reactions	Ref.	DISCUSSION
24. $Ca(NO_3)_2 \cdot nH_2O$ (cont.)					220-425	Anhydrous salt stable in this region.				
					645	No further weight loss.				
25. $Sr(NO_3)_2$	274 285 421 385	S-S S-S S-L S-L		ST-026	264 550 640	Decomposition measureable at this temperature. Decomposition temperature reported by Oza (ST-026, LE-005) Oxide formation	Not given by Stern or Lee.	$Sr(NO_3)_2 \rightleftharpoons SrO + NO + NO_2$ (48) $Sr(NO_2)_2 + NO_2 \rightleftharpoons Sr(NO_3)_2 + N_2$ (49) $Sr(NO_2)_2 + 2NO \rightleftharpoons Sr(NO_3)_2 + N_2$ (50) $SrO + 2NO_2 + \frac{1}{2}O_2 \rightleftharpoons Sr(NO_3)_2$ (51) $NO_2 \rightleftharpoons NO + \frac{1}{2}O_2$ (52)	ST-026 LE-005	Stern and Lee both comment on the work of Oza and Patel. Both the gas phase and the condensed phases were analyzed. The mechanism in (48) through (52) was proposed. The equilibria in (50) and (51) are apparently quite temperature dependent. Oza pointed out that for (51) the equilibrium is on the side of nitrate formation up to 640° and oxide formation above that temperature. Stern remarked that for an earlier decomposition study carried out at temperatures up to 369, no N_2 formation was reported He concluded that reaction (50) does not become important until higher temperatures are reached.
						The kinetics were studied at 420 and 450 where the nitrate is still stable.	When nitrate is stable: NO, NO_2, SrO, $Sr(NO_2)_2$. At higher temperatures: O_2, N_2, NO, NO_2, SrO, and $Sr(NO_2)_2$.	$4Sr(NO_3)_2 \rightleftharpoons 2Sr(NO_2)_2 + 2SrO + 2NO + N_2$ (53) $Sr(NO_3)_2 \rightleftharpoons Sr(NO_2)_2 + \frac{1}{2}O_2$ (54)	LE-005 ST-026	The kinetic study of Protsenko and Bordyushkova was discussed by Lee and Stern. The overall reaction was reported as (53) while (54) was proposed to account for the presence of oxygen in the reaction products. This differs from the work of Oza who proposed that oxygen was produced by the dissociation of NO_2 as in reaction (52).
26. $Sr(NO_3)_2$	645	S-L	10.65	LA-003 ST-026	615,672	Stern cited these temperatures as those reported by different authors for the beginning of decomposition as evidenced by (cont.)			ST-026	Stern reported that there was disagreement on the temperature of both the melting point and the beginning of decomposition. He found no detailed studies on the decomposition of the anhydrous salt published up to1964.
	618	S-L		ST-026						
	605	S-L		ST-026						
	605 570 645	S-L S-L S-L		LA-011						

	TRANSITIONS				DECOMPOSITION					
COMPOUND	T(°C)	Type	ΔH(kcal/mole)	Ref.	T(°C)	Method/Comments	Products	Reactions	Ref.	DISCUSSION
26. $Sr(NO_3)_2$ (cont.)						bubbles appearing in the melt.				
						TGA was used to study the decomposition of the anhydrous salt at a heating rate of 6-9°/minute.	None given.	None given.	SH-017	Calcium and barium nitrates were also studied in this work. The decomposition temperature for the strontium salt should be between that for the calcium and barium salts. Shargorodskii found, however, that strontium nitrate decomposed at a higher temperature than either calcium or barium.
					580-600	Decomposition temperature				
						TGA was used at a heating rate of 5°C/minute. Gaseous products were removed by a flowing stream of nitrogen.	None given.	None given.	LA-011	Lazarini proposed the same course of reaction as that described for the decomposition of calcium nitrate: some decomposition before the melting point, melting with decomposition, and crystallization of the oxide. The fact that decomposition occurred before the melting point was suggested to account for the discrepancies in reported melting points.
					480	First noticeable weight loss.				
					680	Constant weight. Isothermal measurements of weight loss vs. time were made at 480, 500, 520 and 540.				
						TGA was used at a heating rate of 5.4°C/minute. Reaction products were removed in a slow stream of air. Thermal effects were noted at the following temperatures.	None given.	None given.	WE-021	The composition of the solid phase stable in the range 440-510 is unknown. The percent weight loss did not correspond to either formation of the nitrite or a basic nitrate. It is interesting to note that Lazarini reported no weight loss up to 480, but he did cite the work of an earlier publication according to which slow decomposition was noted at 280°
					280	Anhydrous salt stable to this temperature.				
					280-440	Rapid weight loss.				
					440-510	Constant weight of unknown composition.				
					645	No further weight loss, oxide formed.				

COMPOUND	TRANSITIONS				DECOMPOSITION					DISCUSSION
	T(°C)	Type	ΔH(kcal/mole)	Ref.	T(°C)	Method/Comments	Products	Reactions	Ref.	
26. $Sr(NO_3)_2$ (cont.)						DTA was used to study the decomposition. The heating rate was 15°C/minute. Temperatures for endotherms were 620 and 726.	Nitrous fumes.	None given.	GO-014	A physical description of decomposition was given for calcium, strontium and barium nitrates. At temperatures up to 50° above the melting point bubbling occurs. About 50° above the temperature of first visible bubbling, decomposition to the oxide and nitrogen oxides occurs accompanied by a strong endotherm and rapid evolution of nitrous fumes.
					618	Fusion				
					635	Slight evolution of brown nitrous fumes.				
					672	Vigorous bubbling.				
					715	Rapid evolution of brown nitrous fumes.				
27. $Ba(NO_2)_2$	203 230 262-284	S-S S-S S-L		ST-026	250	Decomposition has been noted as low as this temperature.	At low temperatures, mostly NO and a little N_2. At temperatures high enough for the nitrate to decompose NO_2 and O_2 are also formed.	$Ba(NO_2)_2 \rightleftarrows BaO + NO_2 + NO$ (55) $Ba(NO_2)_2 + 2NO_2 \rightleftarrows Ba(NO_3)_2 + 2NO$ (56) $BaO + 3NO \rightleftarrows Ba(NO_2)_2 + \frac{1}{2}N_2$ (57) $Ba(NO_3)_2 \rightleftarrows Ba(NO_2)_2 + O_2$ (58)	ST-026 LE-005	Decomposition has been observed as low as 250°C, which is probably why there is wide disagreement in reported values for the melting point. Rate studies at 410-440°C showed rate to vary in the order air > vacuum > argon.
					400	The reaction between BaO and NO_2 becomes important above this temperature.				
					525	The nitrate begins to slowly decompose at this temperature.				
						The decomposition was studied over the range 400-550. The effects of time, mass of starting material, and addition of nitrate were also studied.	At 400° the products are mostly NO with some NO_2 and N_2. At 550° the amount of NO_2 increases.	See reactions 55-58.	OZ-002	This work was reviewed by Lee and Stern, but many of the results were not discussed. Oza concluded that the reactions occur in the melt since with increased mass of starting material more nitrate is produced and less nitrogen oxides are produced. Reaction (57) was proposed as the method of N_2 production with the reaction occurring mainly in the melt. Reaction (57) was found to take place at 200°C.
					400	Reaction is slow.				
					550	Nitrate decomposition becomes important.				
					(cont.)	(cont.)	(cont.)	(cont.)	(cont.)	(cont.)

COMPOUND	TRANSITIONS				DECOMPOSITION					DISCUSSION
	T(°C)	Type	ΔH(kcal/mole)	Ref.	T(°C)	Method/Comments	Products	Reactions	Ref.	
27. $Ba(NO_2)_2$ (cont.)						A TGA study under vacuum was carried out from 90 to 700°C. Gases were removed from the condensed phase. The solid products were studied using I R methods. The following was found.	Gaseous products not analyzed.	$2Ba(NO_2)_2 \rightleftarrows Ba(NO_3)_2 + BaO + \frac{1}{2}N_2$ (59) $Ba(NO_3)_2 \rightleftarrows BaO + 2NO_2 + \frac{1}{2}O_2$ (60)	PA-013	These studies were performed under nonequilibrium conditions with gaseous products removed. Reaction (59) is just the sum of 2 times (55) plus (56) plus (57). Reaction (60) was proposed for nitrate decomposition but was not verified experimentally.
					90-150	Nitrate formation with stoichiometry as in reaction (59).				
					150-450	Constant weight.				
					450-600	Weight loss, oxide formation according to proposed reaction (60).				
						The reaction between N_2O_4 and $Ba(NO_2)_2$ was studied below 350 and that of N_2O_4 + BaO below 500. The duration of each reaction was 30 minutes.		$Ba(NO_2)_2 + 2N_2O_4 \rightarrow Ba(NO_3)_2 + 2N_2O_3$ (61) $BaO + 4NO_2 \rightarrow Ba(NO_2)_2 + Ba(NO_3)_2$ (62)	OZ-007	Reactions (61) and (62) should also be considered in the mechanism for nitrite decomposition since they might take place in the melt. The nitrite reaction is not appreciable until 300 and the oxide reaction becomes appreciable at 200.
28. $Ba(NO_3)_2$	593 588	S-L S-L	6.0	LA-008 GO-014	525-550	Slow decomposition has been observed in this temperature range.		$Ba(NO_3)_2 \rightleftarrows Ba(NO_2)_2 + O_2$ (58) overall: $Ba(NO_3)_2 \rightleftarrows BaO + 2NO_2 + \frac{1}{2}O_2$ (60)	ST-026	Decomposition of the liquid just above the melting point is slow. Decomposition pressures for (60) were calculated by Stern up to 800°K and extrapolated to 1100°K and by Kelley (KE-021).
						DTA was used to study the decomposition of barium nitrate. The following were noted.	None given.	None given.	GO-014	The value for melting temperature is lower than the value reported in several compilations. No decomposition was noticed up to 588, which is in disagreement with the work of Oza (OZ-005) who reported nitrite formation at 525.
					< 587	No thermal effects.				
					588	Fusion (cont.)	(cont.)	(cont.)	(cont.)	(cont.)

	TRANSITIONS				DECOMPOSITION					
COMPOUND	T(°C)	Type	ΔH(kcal/mole)	Ref.	T(°C)	Method/Comments	Products	Reactions	Ref.	DISCUSSION
28. $Ba(NO_3)_2$ (cont.)					605	Slight bubbling.				
					661	Slight evolution of nitrous fumes (NO_2).				
					692	Rapid evolution of nitrous fumes (NO_2).				
						TGA was used to study the decomposition at a heating rate of 6-9°C/minute.	Not given.	None given.	SH-017	Barium nitrate began to decompose before strontium nitrate according to this study.
					555-600	This was established as the decomposition temperature.				
						TGA was used to study the decomposition. Reaction products were removed by a nitrogen stream. Some isothermal rate measurements were carried out at 460, 480 and 500.	BaO, BaO_2	None given.	LA-011	BaO_2 is still stable at 500 in N_2 and 540 in O_2, and it is always the reaction product. The BaO which results is oxidized by the O_2 produced from NO_2 dissolution. The rate of decomposition was said to be limited by transfer of gas bubbles through the gas-solid interface.
					495	Decomposition temperature in N_2 atmosphere.				
					540	Decomposition temperature in O_2 atmosphere.				
29. Titanium Nitrite										No evidence for the existence of this compound was found.
30. $Ti(NO_3)_4$	58	S-L		ST-026	58	Stable at least up to this temperature.	TiO_2, NO_2 O_2	None given	ST-026	
31. Vandium Nitrite										No evidence was found for the existence of this compound.

	TRANSITIONS				DECOMPOSITION					
COMPOUND	T(°C)	Type	ΔH(kcal/mole)	Ref.	T(°C)	Method/Comments	Products	Reactions	Ref.	DISCUSSION
32. Vanadium Nitrate										No evidence was found for the existence of this compound.
33. Chromium Nitrite										No evidence for the existence of this compound was found.
34. $Cr(NO_3)_3$						TGA was used in a vacuum and in N_2 atmosphere.	Cr_2O_3	None given.	ST-026	Stern reports that although no stable intermediate was observed below 200°C in the thermogram, the decomposition may have involved a series of unstable oxide nitrates
					60	Rapid decomposition begins.				
					100	The rate of decomposition is greatest at this point.				
					200	The first plateau corresponding to Cr_2O_3 was reported at this temperature.				
35. $Cr(NO_3)_3 \cdot 9H_2O$					96	Lowest sample temperature at which HNO_3 vapors were observed.	Spectrometric analysis of gaseous products showed traces of HNO_3, the concentration of which increased with increasing temperature.	None given.	KA-022	
					< 120	First endothermic effect caused by the melting of the salt in its water of crystallization.				
					120-160	Interval during which second endothermal effect occurs. This is due to the simultaneous boiling of the melt and decomposition of the nitrate.				
					130	Maximum concentration of HNO_3 vapors (4.76%) recorded at this temperature.				

COMPOUND	TRANSITIONS				DECOMPOSITION					DISCUSSION
	T(°C)	Type	ΔH(kcal/mole)	Ref.	T(°C)	Method/Comments	Products	Reactions	Ref.	
35. $Cr(NO_3)_3 \cdot 9H_2O$ (cont.)						TGA apparatus was employed in this study with a linear heating rate of 5.4°C/min. A slow stream of air was passed through the furnace.	Analysis of the gas phase was not carried out.	None given.	WE-021	In the interval 250-380°C a plateau was reached in the thermogram. The composition of this phase was unknown; however, the author states that it did not correspond to a basic nitrate.
					55	Salt began to lose water of hydration.				
					55-250	A rapid weight loss was observed in this range.				
					250-380	Constant weight.				
					380-445	Further weight loss.				
					445	Constant weight Cr_2O_3 formed.				
						Decomposition to a basic nitrate was carried out in presence of reducing agent such as alcohol or acetone to prevent conversion of Cr(III) to Cr(VI).	$Cr_n(OH)_{3n-1}NO_3$ HNO_3, H_2O	$nCr(NO_3)_3 \cdot 9H_2O \rightarrow Cr_n(OH)_{3n-1}NO_3 + (3n-1)HNO_{3(g)} + (6n+1)H_2O_{(g)}$ (63)	MA-042	The author stated that nitrate decomposition proceeds via hydroxynitrate intermediates. By not allowing the decomposition to go to completion, the stable intermediates were identified.
36. Manganese Nitrite										No evidence for the existence of this compound was found.
37. $Mn(NO_3)_2$					~160	Decomposition begins.	MnO_2 NO_2	$Mn(NO_3)_2 \rightleftarrows MnO_2 + 2NO_2$ (64)	ST-026 DE-024	Stern reported that conflicting opinions exist on the type of bonding in the molecule. Addison and Gatehouse (AD-004) characterized it as cavalent, but Dehnicke and Straehle (DE-024) reported that the salt had considerable ionic character. Some disagreement also exists on the composition of the oxide produced by thermal decomposition. Stern gives reaction (64)
					180	Another study at 10^{-4} mm Hg resulted in this decomposition temperature.	$MnO_{1.8}$			
					230	Rate of decomposition is greatest at this temperature when reaction is carried out in an atmosphere of dry N_2.				

COMPOUND	TRANSITIONS				DECOMPOSITION					DISCUSSION
	T(°C)	Type	ΔH(kcal/mole)	Ref.	T(°C)	Method/Comments	Products	Reactions	Ref.	
37. $Mn(NO_3)_2$ (cont.)					≥ 50	Some decomposition of the nitrate occurs.			KA-023	Absorption of NO_2 by MnO_2 was studied. The results showed that the absorption efficiency decreased with increasing temperature due to product decomposition beginning at 50°C.
38. $Mn(NO_3)_2 \cdot 4H_2O$	37.1	S-L		RO-007		TGA study of stability and kinetics in static air.		$Mn(NO_3)_2 \cdot 4H_2O \rightarrow Mn(NO_3)_2 \cdot 2H_2O + 2H_2O$ (65)	LU-011	Lumme and Raivio (LU-011) stated that during investigations of n-hydrates carried out by Duval (DU-009) and Dubois (DU-007, DU-008), no stable intermediate hydrates were detected. Dubois found an intermediate impure dioxide MnO[illegible] at 280-300°C, which changed to Mn_2O_3 and Mn_3O_4 at higher temperatures. Duval reported the product at 700°C as Mn_3O_4. The activation energies for reaction (65), (66), and (67) were reported to be 9.3 ± 0.3, 23.7 ± 0.5, and 45.7 ± 2 kcal/mole respectively.
					50-184	16.6% measured weight loss corresponding to partial dehydration.	$Mn(NO_3)_2 \cdot 2H_2O$			
					184-279	Weight loss (58.5%)	MnO_2, H_2O, NO_2	$Mn(NO_3)_2 \cdot 2H_2O \rightarrow MnO_2 + 2H_2O + 2NO_2$ (66)		
					279-528	Constant weight.				
					528-635	Weight loss, (10.2%).	Mn_2O_3, O_2	$MnO_2 \rightarrow \frac{1}{2}Mn_2O_3 + \frac{1}{4}O_2$ (67)		
						A pyrolysis study in a "normal atmosphere" gave the following results:			LU-011 (HE-014)	This investigation was done by Hegedüs (HE-014) and reviewed by Lumme and Raivio (LU-011). No stable intermediate hydrate was detected in this study. The MnO_2 stable temperature range was found to be lower than that reported in reference (LU-011).
					50-230	Decomposition of tetrahydrate during this temperature interval.	β-MnO_2			
					450-580	Further decomposition.	α-Mn_2O_3			
39. $Mn(NO_3)_2 \cdot 6H_2O$	25.8	S-L	9.61	MA-025 RO-007 LA-008	22-51	Melting of the nitrate in its water of crystallization.	Spectrometric analysis of gaseous products showed traces of HNO_3, the concentration of	None given.	KA-022	
					117-61	Boiling of the melt occurred along with partial removal of the water.				
					(cont.)	(cont.)	(cont.)	(cont.)	(cont.)	(cont.)

	TRANSITIONS				DECOMPOSITION					
COMPOUND	T(°C)	Type	ΔH(kcal/mole)	Ref.	T(°C)	Method/Comments	Products	Reactions	Ref.	DISCUSSION
39. $Mn(NO_3)_2\cdot 6H_2O$ (cont.)					145	Temperature at which first HNO_3 vapors were observed.	which increased with increasing temperature.	None given.	KA-022	
					186	Decomposition of the sample became intensive, followed by cooling to 168.				
					215	Temperature at which maximum concentration of HNO_3 vapors recorded (1.16%).				
								$Mn(NO_3)_2\cdot 6H_2O_{(\ell)} \rightleftharpoons MnO_2 + 2NO_2 + 6H_2O_{(\ell)}$ (68) $Mn(NO_3)_2\cdot 6H_2O_{(\ell)} \rightleftharpoons MnO_2 + 2NO_2 + 6H_2O_{(g)}$ (69)	KE-021	Using heats of formation reported in the literature, Kelley calculated overall heats of decomposition (reactions 68 and 69) at 298.2°K. He also estimated free energies and equilibrium pressure-temperature relationships associated with the same reactions.
40. Ferrous Nitrite										No evidence for the existence of this compound was found.
41. Ferrous Nitrate, Anhydrous										No evidence for the existence of this compound was found.
42. $Fe(NO_3)_2\cdot 6H_2O$	60.5	S-L		RO-007						No information concerning the decomposition of this compound was found
43. Ferric Nitrite										No evidence was found for the existence of this compound.
44. $Fe(NO_3)_3$	35-100	S-L		AN-008	100-250	Sample decomposed over this range in a DTA study.			AN-008	DTA analysis of catalyst mixtures gave these results. The article was not available in English, and the identity of the compound for which these data were reported is questionable.
					(cont.)	(cont.)	(cont.)	(cont.)	(cont.)	(cont.)

	TRANSITIONS				DECOMPOSITION					
COMPOUND	T(°C)	Type	ΔH(kcal/mole)	Ref.	T(°C)	Method/Comments	Products	Reactions	Ref.	DISCUSSION
44. $Fe(NO_3)_3$ (cont.)					Room Temperature	Slow decomposition occurs.			LO-014	This investigation was the first successful attempt to isolate the compound. It was reported to be a yellow-brown involatile solid having low thermal stability. Stern (ST-026) reported that anhydrous ferric nitrate had only been prepared as the volatile adduct $Fe(NO_3)_3\cdot N_2O_4$, although $Fe(NO_3)_3$ might exist in the vapor state.
					~ 70	Rapid decomposition occurs under reduced pressure.	Fe_2O_3	--		
45. $Fe(NO_3)_3\cdot 9H_2O$	50.1	S-L		RO-007		The stability and kinetics of decomposition were studied using TGA with a heating rate of 330°C/hr. in an atmosphere of static air.			LU-010	Lumme and Junkkarinen (LU-010) reported an activation energy of 14.7 ± 0.6 kcal/mole and a reaction order of 0.55 for reaction (71).
					50-139	Partial dehydration occurs (18.9 % wt. loss.)	$Fe(NO_3)_3\cdot 5H_2O$	$Fe(NO_3)_3\cdot 9H_2O \rightarrow Fe(NO_3)_3\cdot 5H_2O + 4H_2O$ (70)		
					139-405	Further weight loss (74.4%).	αFe_2O_3, NO_2, O_2, and H_2O	$Fe(NO_3)_3\cdot 5H_2O \rightarrow \frac{1}{2}Fe_2O_3 + 5H_2O + 3NO_2 + \frac{3}{4}O_2$ (71)		
					405-850	Constant weight.				
					84	First HNO_3 vapors were detected.	Spectrometric analyses of gaseous products showed traces of HNO_3 vapors.	None given.	KA-022	The HNO_3 observed at 84°C could have been an impurity attached to the original sample and does not necessarily mean that nitrate decomposition had begun
					<120	Endothermic effect due to melting of the salt in its water of crystallization.				
					120-160	Interval during which simultaneous boiling of the melt and decomposition of the nitrate occurred.				
					163.5	Greatest HNO_3 vapor concentration (11.52%) was observed at this point.				
					(cont.)	(cont.)	(cont.)	(cont.)	(cont.)	(cont.)

	TRANSITIONS				DECOMPOSITION					
COMPOUND	T(°C)	Type	ΔH(kcal/mole)	Ref.	T(°C)	Method/Comments	Products	Reactions	Ref.	DISCUSSION
45. $Fe(NO_3)_3 \cdot 9H_2O$ (cont.)						TGA study employing a heating rate of 5.4°C/min. A slow stream of air removed the gaseous products. The following thermal effects were observed:		None given.	WE-021	This investigator, in contrast to Lumme (LU-010), did not observe a stable intermediate hydrate or anhydrous nitrate.
					35	Salt began to lose water of hydration.				
					445	Constant weight achieved.				
						This TGA study in air was carried out in two parts: I. Programmed heating rate of 5.6°C/min., and II: Extended run lasting ~ 84 hours over a 430° temperature span.		$3NO_2 + H_2O \rightarrow 2HNO_3 + NO$ (72)	KE-026	This behavior of this compound was described as unique in that no red-brown NO_2 fumes were detected. The author proposed that the NO_2 formed, if any, reacted with excess water vapor according to reaction (73). No stable intermediate was detected in either run. The final product was analyzed by X-ray diffraction; the result was in agreement with all other studies with the exception of that of Duval (DU-010) discussed below. Note the lower decomposition temperature with application of the slower heating rate.
						Run I (20 to 1040°C):				
					100-150	Weight loss began during this interval.				
					250	Decomposition approaching completion				
					350	Constant weight as shown on thermogram.	α-Fe_2O_3			
						Run II (20-450°C):				
					20-100	Weight loss began during this interval.				
					200	Decomposition fairly complete.				
					215-450	1.1% weight loss recorded during this interval.	α-Fe_2O_3			
					38	Begins to lose water of crystallization.	H_2O, NO_2	None given	DU-010	The final product reported by Duval is in disagreement with the results of other investigators (KE-026,
					(cont.)	(cont.)	(cont.)	(cont.)	(cont.)	(cont.)

	TRANSITIONS				DECOMPOSITION					
COMPOUND	T(°C)	Type	ΔH(kcal/mole)	Ref.	T(°C)	Method/Comments	Products	Reactions	Ref.	DISCUSSION
45. $Fe(NO_3)_3 \cdot 9H_2O$ (cont.)					120	Red fumes given off. Decomposition begins.			DU-010	LU-010, WE-021). The temperature at which constant weight is reached is ~ 100-150 degrees lower than that reported in several of the studies (LU-010, WE-021) although in fair agreement with the third (KE-026).
					144	Reaction becomes intense.				
					160	Reaction slows down as it approaches this temperature. Last traces of nitrogen oxides observed.				
					311-1000	Constant weight.	Fe_3O_4			
46. $Co(NO_3)_3$					~100	Decomposition begins	NO_2		ST-026	Stern regards the existence of this compound as doubtful.
47. $Co(NO_3)_2$					100-105	Decomposition begins.	Co_3O_4	None given.	ST-026	No intermediate is formed in the decomposition.
					~170, 270	Conflicting reported temperatures at which rate of decomposition is a maximum.				
					180	Decomposition in a vacuum occurs at this temperature.	Co_3O_4, NO_2, O_2		DE-024	
48. $Co(NO_3)_2 \cdot 6H_2O$	-33 20 57	S-S S-S S-L	1.7 0.7	PO-012 PO-012 RO-007		DTA study carried out with 0.1-0.15 g samples. Heating rate was 15-17°C/min. The following thermal effects were observed:		None given.	SA-026	Note that the thermal effect at 150-180°C reported in this investigation corresponds to the decomposition temperature for the anhydrous salt reported by Dehnicke and Straehle (DE-024). No explanation was made in the abstract for the effect at 250-80. It was also reported that an exothermic effect occurred but the abstract does not state at what temperature it took place.
					55-60	Melting in water of crystallization.				
					150-180	Evolution of gaseous product.	NO_2			
					250-280	Endothermal effect.				
					280-800	Final product is stable.	Co_3O_4			
					(cont.)	(cont.)	(cont.)	(cont.)	(cont.)	(cont.)

	TRANSITIONS				DECOMPOSITION					
COMPOUND	T(°C)	Type	ΔH(kcal/mole)	Ref.	T(°C)	Method/Comments	Products	Reactions	Ref.	DISCUSSION
48. Co(NO$_3$)$_2$ ·6H$_2$O (cont.)						The decomposition was studied under air and dynamic nitrogen atmospheres using TGA. The average heating rate was ~ 5.5°C/min. In air, the thermogram showed the following:			LU-009	This study also generated the activation energies for reaction (73) in static air and dynamic nitrogen atmospheres. They are 9.7 ± 1 and 11.4 ± 1 kcal/mole respectively. After losing all its water of hydration between 50 and 233°C, the salt decomposed directly to Co$_3$O$_4$.
					50-233	38.7% weight loss.	Co(NO$_3$)$_2$, H$_2$O,	Co(NO$_3$)$_2$ · 6H$_2$O - Co(NO$_3$)$_2$ + 6H$_2$O (73)		
					233-280	52.6% weight loss.	Co$_3$O$_4$, NO$_2$, O$_2$	Co(NO$_3$)$_2$ - $\frac{1}{3}$Co$_3$O$_4$ + 2NO$_2$ + $\frac{1}{3}$O$_2$ (74)		
					280- ~ 800	Constant weight.				
						The nitrogen atmosphere thermogram was similar:				
					<50-227	34.2% weight loss.	Co(NO$_3$)$_2$, H$_2$O	Reaction (73)		
					227-315	54.9% weight loss.	Co$_3$O$_4$, NO$_2$, O$_2$	Reaction (74)		
					315- ~ 800	Constant weight.				
					22-51	Endothermal effect due to melting of the nitrate in the water of crystallization.	Spectrometric analysis of gaseous products showed traces of HNO$_3$ vapors.		KA-022	This study was reviewed by Lumme and Junkkarinen (LU-009) who reported similar results.
					118-51	Endothermic effect caused by boiling of the melt with removal of part of the water of crystallization.				
					138	First appearance of HNO$_3$ vapors.				
					190-245	Intense decomposition.				
					217.5	Temperature at which greatest concentration				
					(cont.)	(cont.)	(cont.)	(cont.)	(cont.)	(cont.)

	TRANSITIONS				DECOMPOSITION					
COMPOUND	T(°C)	Type	ΔH(kcal/mole)	Ref.	T(°C)	Method/Comments	Products	Reactions	Ref.	DISCUSSION
48. Co(NO$_3$)$_2$ ·6H$_2$O (cont.)						of HNO$_3$ vapors (4.98%) was recorded.				
					235-40	Unexplained thermal effect.				
						TGA was used to study this compound. The heating rate was 5.4° C/min. A slow stream of air was passed through the furnace.		None given	WE-021	Wendlandt reported no intermediate breaks in the decomposition curve. He also noted that the minimum oxide level temperature for cobalt nitrate was the lowest of all 15 compounds studied. His results are similar to those given by Lumme (LU-009).
					50	Dehydration begins.				
					290	Oxide level reached.	Co$_3$O$_4$			
						TGA was used for two types of runs in air. Type I runs were programmed runs at a heating rate of 5.8°C/min. from 20 to 1040°C. Type II was an extended run lasting 53 hours from 20-350°C.	NO$_2$, H$_2$O Co$_3$O$_4$		KE-026	Constant weight is not achieved at any stage before complete decomposition to cobalto-cobaltic oxide. An increase in time, or slower heating rate, was found to lower the decomposition temperature.
						Type I Run:				
					350	Decomposition to Co$_3$O$_4$ complete.				
						Type II Run:				
					150	Red-brown fumes.				
					210	Decomposition complete.				
49. Ni(NO$_3$)$_2$					220	Temperature at which decomposition in vacuum occurs.			ST-026 AD-005	This compound is reported to be slightly volatile. It is prepared by reaction of nickel carbonyl with gaseous N$_2$O$_4$. Addison (AD-005) states that reaction of the carbonyl with liquid N$_2$O$_4$ results in formation of the nitrate.
					260	Compound is stable in an argon atmosphere up to this temperature.				
50. Ni(NO$_2$)$_2$					260	Decomposition begins at this temperature.	Ni(NO$_3$)$_2$		ST-026	
					105	Decomposition occurs.	NiO		KA-014	Kalinchenko, without citing a reference, (cont.)

	TRANSITIONS				DECOMPOSITION					
COMPOUND	T(°C)	Type	ΔH(kcal/mole)	Ref.	T(°C)	Method/Comments	Products	Reactions	Ref.	DISCUSSION
50. $Ni(NO_3)_2$ (cont.)										reports that decomposition occurs at a much lower temperature than that reported by Stern (ST-026). He also states that disagreement exists concerning the temperature ranges which correspond to the various phases and the composition of the phases.
51. $Ni(NO_3)_2 \cdot 6H_2O$	56.7	S-L		RO-007		DTA was carried out with 0.1-0.15 g samples. Rate of heating was 15-17°C/min. up to 800°C. The thermogram showed 5 peaks:			SA-026	
	50	S-L		SA-026						
	55	S-L		KA-014						
					50	Melting in water of crystallization.				
					136.7	Dehydration	$Ni(NO_3)_2 \cdot 3H_2O$			
					270,275, 340	Further dehydration takes place.				
					800	Final product identified.	NiO			
						TGA study carried out in air in two parts: I. Programmed run employing a heating rate of 5-6°C/min. from 20 to 4010°C.			KE-026	The slower heating rate resulted in lower decomposition temperatures and the formation of a stable intermediate not detected in the temperature programmed run. The author states that evolution of NO_2 fumes prior to 250°C suggests that nitrate decomposition starts before 4 moles of water are evolved.
					200	Weight loss corresponding to slightly more than one H_2O.	H_2O			
					<250	Red brown fumes	NO_2			
					400	Decomposition essentially complete.	NiO			
					>400	Constant weight.				
						II. Extended run lasting 77 hours, 36 minutes from				
					(cont.)	(continued)	(cont.)	(cont.)	(cont.)	(cont.)

	TRANSITIONS				DECOMPOSITION					
COMPOUND	T(°C)	Type	ΔH(kcal/mole)	Ref.	T(°C)	Method/Comments	Products	Reactions	Ref.	DISCUSSION
51. $Ni(NO_3)_2 \cdot 6H_2O$ (cont.)						20 to 450°C.				
					210	Stable Ni compound.	Possibly nickel basic nitrate with 1½ moles H_2O.			
					300	Decomposition essentially complete.	NiO, NO_2, H_2O			
						DTA was used in a water vapor-air atmosphere. Heating rate was 5-7°C/min. The melt was analyzed after each thermal effect. Gaseous products were analyzed.		$Ni(NO_3)_2 \cdot nH_2O \rightarrow xNi(NO_3)_2 \cdot yNi(OH)_2 \cdot zH_2O \rightarrow NiO$ (75)	KA-013 KA-014 PU-002	The nitric acid vapors evolved from 127 to 164 were reported to have been an impurity in the starting material. The author states that the evolution of this impurity was what Karavaev and Kirillov (KA-022) observed in their studies of the hydrated nitrates of Al, Cr, Fe, Mn, Co and Ni. The fact that Ni_2O_3 was not detected in the reaction products was in contrast with other findings reviewed by the author.
					55	Melting in water of crystallization.				
					10	Loss of 0.2 moles water.				
					127-64	Unstable tetrahydrate color change from bluish green to emerald green.	HNO_3			
					170	Trihydrate				
					190,210 235	Endothermal effects marking the beginning of nitrate decomposition and further loss of water.				
					257	Vigorous decomposition of nitrate. Yellow green mass.	$Ni(NO_3)_2 \cdot 1.16Ni(OH)_2$			
					310-37	Decomposition of the hydroxide-nitrate	NiO			

COMPOUND	TRANSITIONS T(°C)	Type	ΔH(kcal/mole)	Ref.	DECOMPOSITION T(°C)	Method/Comments	Products	Reactions	Ref.	DISCUSSION
51. $Ni(NO_3)_2 \cdot 6H_2O$ (cont.)						TGA was used in a slow stream of air. Gaseous products were not analyzed.	NiO	None given	WE-021	Only one stable hydrate intermediate was observed.
					50	Loss of water of hydration.				
					50-205	Rapid weight loss.				
					205	Formation $Ni(NO_3)_2$				
					>205	Rapid weight loss				
					505	Constant weight.				
						Experimental details not given in abstract.	Spectrophotometric analysis of gaseous products showed traces of HNO_3 vapors	None given	KA-022	
					32-51	Melting in water of hydration.				
					127-162	Partial dehydration				
					138	Observation of HNO_3 vapors.				
					162-259	Decomposition of nitrate.				
					235	Greatest concentration of HNO_3 vapors observed.				
					290-337	Unexplained thermal effect.				
52. $CuNO_2$										No evidence for the formation of this compound was found in the literature.
53. $CuNO_3$										No evidence for the formation of this compound was found in the literature.
54. $Cu(NO_2)_2$										Stern (ST-026) states that there are conflicting reports concerning the existence of this compound.

COMPOUND	TRANSITIONS T(°C)	Type	ΔH(kcal/mole)	Ref.	DECOMPOSITIONS T(°C)	Method/Comments	Products	Reactions	Ref.	DISCUSSION
55. $Cu(NO_3)_2$	255	S-L		ST-026	<227	Vaporization of the solid salt. Only the solid phase undergoes decomposition in this range.	NO_2, O_2	None given.	ST-026	Stern reports that the vapor pressure of $Cu(NO_3)_2$ has been determined.
	180-200	S-G	15.6		>227	Both solid and vapor decompose above this temperature.				
					325-75	Range of study in equimolar melt of $NaNO_3$-KNO_3.	CuO, NO_2, O_2	$Cu^{++} + NO_3^- \rightleftharpoons CuO + NO_2^+$ (76) $NO_2^+ + NO_3^- \rightleftharpoons 2NO_2 + \frac{1}{2}O_2$ (77)	KU-012	The mechanism and kinetics of decomposition in alkali metal melts were studied. CuO was found to catalyze reaction (77). The author concluded that possibly CuO might catalyze any acid-base reaction in nitrate solvents where NO_2^+ ion is the …termediate species. Other metal oxides might act similarly.
56. $Cu(NO_3)_2 \cdot 3H_2O$						This study was carried out by means of TGA at a heating rate of 5.5°C/min. in static air.			LU-008	The activation energies for reactions (78) and (79) were calculated to be 13.2 ± 2 and 48.4 ± 2 kcal/mole respectively. The reaction orders were also determined. Some disagreement exists concerning the composition of the intermediate as reported in earlier papers. Lumme and Junkkarinen (LU-008) state that most investigators agree that some sort of basic nitrate is formed at 250 having a composition of either $Cu(NO_3)_{0.5}OH_{1.5}$ or $Cu(NO_3)(OH)$. However Keely and Manor (KE-026) report no basic intermediate formation.
					86-250	39.7% weight loss.	$Cu(NO_3)OH$ HNO_3 H_2O	$Cu(NO_3)_2 \cdot 3H_2O \rightarrow Cu(NO_3)OH + HNO_3 + 2H_2O$ (78)		
					250	Basic salt formed.				
					250-305	46.8% weight loss.	CuO	$Cu(NO_3)OH \rightarrow CuO + HNO_3$ (79)		
					305-550	Thermogram shows nearly constant weight, corresponding to CuO formation.				
						TGA was used in two types of experiments. I. (from 20 to 1040):			KE-026	Decomposition was completed at a lower temperature when the heating rate was considerably reduced. No evidence for the formation of an oxynitrate was found.
					200-250	Most of water loss occurred during this interval.	H_2O, CuO, NO_2			
					(cont.)	(cont.)	(cont.)	(cont.)	(cont.)	(cont.)

	TRANSITIONS				DECOMPOSITION					
COMPOUND	T(°C)	Type	ΔH(kcal/mole)	Ref.	T(°C)	Method/Comments	Products	Reactions	Ref.	DISCUSSION
56. $Cu(NO_3)_2 \cdot 3H_2O$ (cont.)					350	Decomposition essentially complete.				
						II. (from 20 to 350):				
					210	Decomposition complete				
						The decomposition in a slow stream of air was studied using TGA with a heating rate of 5.4°C/min. The gaseous products were not analyzed.		None given.	WE-021	This investigator also reported the formation of a basic nitrate intermediate, although different in composition from those mentioned above.
					70	Salt began to dehydrate.				
					70-165	Rapid weight loss.				
					165	Break in the curve corresponding to a basic nitrate.	$Cu_2O(NO_3)_2$			
					165-325	Further decomposition was observed.				
					325	CuO level.	CuO			
						DTA was employed by this investigator. No attempt was made to analyze products or propose mechanisms. The heating rate was ~ 15°C/min.			GO-014	
					120	Dissolution.				
					~200	Initial appearence of nitrous fumes.				
					203	Rapid nitrous fumes.				
					310-446	DTA curve showed a change from endothermal to exothermal.				
					> 400	No further visible reaction.				

	TRANSITIONS				DECOMPOSITION					
COMPOUND	T(°C)	Type	ΔH(kcal/mole)	Ref.	T(°C)	Method/Comments	Products	Reactions	Ref.	DISCUSSION
56. $Cu(NO_3)_2 \cdot 3H_2O$ (cont.)					~ 480	Peak of exothermal portion of curve with gradual decrease to 761°C.				
57. $Cu(NO_3)_2 \cdot 6H_2O$	24.4	S-L	8.7	LA-008					LU-008	This paper does not deal directly with the hexahydrate, but rather with the trihydrate. However in a brief discussion of reported intermediates in the decomposition of both salts, the authors stated that formation of the basic salts $Cu(NO_3)_{0.67}(OH)_{1.33}$ and $Cu(NO_3)_{0.5}(OH)_{1.5}$ had been reported. It was also noted that the decomposition behavior of the hexahydrate in air and vacuum is quite different from that of the trihydrate. No further details were given.
58. $AgNO_2$						Weight of sample before and after heating was measured in four different atmospheres.			SC-029 (Divers)	A survey of the literature on $AgNO_2$ decomposition was prepared in 1969 by J. W. Schneller (SC-029). The contents of this survey are given here in chronological order. The earliest study led the investigation to the following conclusions: No AgO was formed. The nitrite decomposed according to reaction (80). If NO_2 is not removed, it reacts with the sample to form $AgNO_3$ and NO.
					85-140	Range of study.				
						I. Unsealed Vessel, restricted air flow.		$AgNO_2 \rightarrow Ag + NO_2$ (80) or $AgNO_2 \rightarrow Ag + NO + \frac{1}{2}O_2$ (81)		
						II. Sealed vessel.		$2AgNO_2 \rightarrow Ag + AgNO_3 + NO$ (82)		
						III. Open vessel.		$3AgNO_2 \rightarrow 2Ag + AgNO_3 + NO_2 + NO$ (83)		
						Decomposition took place in a vacuum; NO_2 evolved was trapped in a chilled receiving flask.	NO_2, NO, $AgNO_3$		SC-029 (Divers & Shimidzu)	These results indicated that $\frac{1}{3}$ of the nitrogen in the original sample went to NO_2, and $\frac{2}{3}$ formed nitrate and nitric oxide. From the information gained in several side experiments, it was concluded that $AgNO_3$ formed from Ag and NO_2. No reaction between
					(cont.)	(cont.)	(cont.)	(cont.)	(cont.)	(cont.)

	TRANSITIONS				DECOMPOSITION					
COMPOUND	T(°C)	Type	ΔH(kcal/mole)	Ref.	T(°C)	Method/Comments	Products	Reactions	Ref.	DISCUSSION
58. $AgNO_2$ (cont.)										silver nitrite and NO_2 was detected even after prolonged contact.
						Samples were heated rapidly in vacuum system.		$AgNO_2 + NO_2 - AgNO_3 + NO$ (84)	SC-029 (Oswald)	Oswald, in contrast to Divers (above), found that $AgNO_2$ and NO_2 do react (84). In addition he studied the rates of decomposition at various temperatures. The solid products of decomposition were found to be predominantly silver, with traces of $AgNO_3$. No silver nitrite was found.
					100	Rate of decomposition was slow.				
					130	Noticeable rate of decomposition.				
					200	Rapid decomposition.				
						I. Study carried out at 195° under vacuum, gaseous products remove.		$AgNO_2 - Ag + NO_2$ (80)	SC-029 (Centerszwer and Checinski)	Under the first set of experimental conditions, reaction (80) went to completion. However, if the gaseous products remained in contact with the sample, the overall reaction was (82), which is the sum of (80) and (84). Reduction of NO_2 to NO was visually observed during the course of the decomposition.
						II. Decomposition carried out under pressure.		$AgNO_2 + NO_2 - AgNO_3 + NO$ (84) $2AgNO_2 - Ag + AgNO_3 + NO$ (82) $Ag + NO_2 - AgNO_2$ (85)		
						Dry NO_2 was passed over $AgNO_2$ for 7 hours at 100°		$AgNO_2 + NO_2 - AgNO_3 + NO$ (84)		Reaction (84) was investigated. A weight increase corresponding to 85.1% of (84) was observed. Attempts to observe the reverse of reaction (84) failed.
						Kinetic measurements of $AgNO_2$ decomposition were made by studying either volume change or pressure change. The composition of the gas was analyzed as a function of pressure.	99.7% NO_2, 0.3% NO at 1 mm. 100% NO at 1 atm.	$AgNO_2 - Ag + NO_2$ (80) $2AgNO_2 - Ag + AgNO_3 + NO$ (82)	SC-029 (Blumenthal & Checinski)	The results of this study along with those of Centnerszwer and Checinski (above) confirmed that (80) occurred in vacuo, while at atmospheric pressure (82) occurred. A combination of these two reactions took place at intermediate pressures. They
					(cont.)	(cont.)	(cont.)	(cont.)	(cont.)	(cont.)

	TRANSITIONS				DECOMPOSITION					
COMPOUND	T(°C)	Type	ΔH(kcal/mole)	Ref.	T(°C)	Method/Comments	Products	Reactions	Ref.	DISCUSSION
58. $AgNO_2$ (cont.)										also found that increasing the pressure resulted in a decreased initial velocity, and that lower decomposition temperatures occurred at lower pressures. They observed an induction period in the interval from 150 to 195° C at constant pressure. Activation energies were measured in this range.
						Microscopic study of decomposition.			SC-029 (Schaum and Becker)	They found that the decomposition varied according to the method by which the crystals were grown.
							Ag, $AgNO_3$, NO	$2AgNO_2 - Ag + AgNO_3 + NO$ (82)	SC-029 (Randall, Manov, and Brown)	A study of the thermodynamics of decomposition at atmospheric pressure according to reaction (82) was carried out by equilibrium vapor pressure measurements. The results confirmed that the activities of $AgNO_2$, Ag, and $AgNO_3$ can be taken as unity. The relative amount of $AgNO_2$ in contact with Ag + $AgNO_3$ was found to have no significant effect on the vapor pressure of NO.
					128	This was reported as the beginning of decomposition of pure $AgNO_2$.	Ag_2O, NO, NO_2	$2AgNO_2 - Ag_2O + NO + NO_2$ (86)	SC-029 (Oza)	Reaction (86) had been proposed by Oza as the "primary stage" of nitrite decomposition. He attempted to detect silver oxide in the decomposition products of both pure $AgNO_2$ and a mixture of $AgNO_2$ and Ag_2O. No Ag_2O was found in either case. He concluded that (82) was the primary stage, but that NO and NO_2 attacked the oxide. In another experiment he was able to isolate Ag_2O by decomposing the nitrite in pure oxygen for 4 hours at 130°C.
							Ag, $AgNO_2$ $AgNO_3$, NO, NO_2.	$AgNO_3 + NO - AgNO_2 + NO_2$ (87) $AgNO_2 + \frac{1}{2}O_2 - AgNO_3$ (88)		A complex scheme of reactions (87-91) was proposed to account for the products found. The silver oxide formed
					(cont.)	(cont.)	(cont.)	(cont.)	(cont.)	(cont.)

	TRANSITIONS				DECOMPOSITION					
COMPOUND	T(°C)	Type	ΔH(kcal/mole)	Ref.	T(°C)	Method/Comments	Products	Reactions	Ref.	DISCUSSION
58. $AgNO_2$ (cont.)								$Ag_2O + NO_2 - Ag_2O_2 + NO$ (89) $Ag_2O_2 \xrightarrow{NO, NO_2} AgNO_2 + AgNO_3$ (90) $Ag_2O + NO_2 - AgNO_2 + Ag$ (91)		in the primary decomposition reaction was said to react with NO to produce mainly $AgNO_2$.
					90	Decomposition temperature.			SC-029 (Boldyrev & Eroshkin, 1964)	The effect of crystal size on the rate of thermal decomposition was investigated. An optimum size was reported. The temperature range studied for decomposition was 70 to 105. At high temperatures the difference in the rate of decomposition between large and small crystals was much less than the difference at low temperatures.
									SC-029 (Boldyrev, & Eroshkin, 1966)	The effect of additives on $AgNO_2$ decomposition was investigated. NiO and Ni_2O_3 were reported to accelerate the reaction; V_2O_5, ThO_2, CdO, and WO_3 had no effect; Ag_2O, CuI, and Li_2O decreased the rate.
						The kinetics of thermal decomposition were studied under vacuum with continuous evacuation. The irradiated and unirradiated samples were placed in a quartz or aluminum boat.	Ag, NO_2		SC-029	This investigation of the kinetics of thermal decomposition of $AgNO_2$ employed both unirradiated and irradiated salts. The decomposition curves were linear in the 15 to 45% weight loss region. The contacting envelope mechanism was verified by microscopic observation, and a kinetically descriptive equation was derived. Exposure to cobalt-60 gamma radiation had an unusual stabilizing effect on the salt; a mechanism was proposed to explain this phenomenon.
					120	Decomposes at this temperature. TGA was used.	Ag, NO_2		ST-026 PA-013	Stern reports that the investigation of the decomposition of this salt is in the preliminary stages. The kinetics
					(cont.)	(cont.)	(cont.)	(cont.)	(cont.)	(cont.)

	TRANSITIONS				DECOMPOSITION					
COMPOUND	T(°C)	Type	ΔH(kcal/mole)	Ref.	T(°C)	Method/Comments	Products	Reactions	Ref.	DISUCSSION
58. $AgNO_2$ (cont.)										are reported to be first-order, and an activation energy of ~ 25kJ/mole has been reported.
					128	$AgNO_2$ begins to decompose forming Ag_2O, NO, and NO_2.	Ag_2O, NO, and NO_2	$2AgNO_2 - Ag_2O + NO + NO_2$ (86)	OZ-006	Oza studied the action of NO_2 on $AgNO_2$ and its decomposition products. Reaction (91) is negligible at 130°C but contributes considerably at higher temperatures. Reaction (86) is not considered to be the true decomposition mechanism by many investigators because no Ag_2O is detected in the reaction products.
					130	$AgNO_2$ oxidized by NO_2 to $AgNO_3$.	$AgNO_3$, and NO	$AgNO_2 + NO_2 - AgNO_3 + NO$ (84)		
					130 and above	Silver oxide reacts with NO_2.		$Ag_2O + NO_2 - AgNO_2 + Ag$ (91)		
59. $AgNO_3$	160	S-S	0.66	RO-007	>127	Ag_2O is very unstable above this temperature.		$2AgNO_3 = Ag_2O + 2NO_2 + \frac{1}{2}O_2$ (92) $2NO_2 = 2NO + O_2$ (93) $2AgNO_3 = 2Ag + 2NO_2 + O_2$ (94) $Ag_2O = 2Ag + \frac{1}{2}O_2$ (95)	ST-026	Stern reports that the decomposition equilibria of this system is complicated by the thermal instability of Ag_2O. Decomposition is reported to be negligible below its melting point, but becomes appreciable above it. Partial pressures for $AgNO_3$ decomposition were calculated at 298, 400, 500, 600, and 700°K. The total pressure at 327°C = 0.209 and at 427°C = 1.94 atm.
			0.609	LA-008						
			0.57	ST-026						
			0.55	AD-002	210	$AgNO_3$ melts.				
	159.4	S-S	0.561	RE-006	240-250	Decomposition becomes appreciable.				
	210	S-L	2.76	JA-013						
	209.6	S-L	2.96	JA-012						
	210	S-L	2.98	ST-026						
	214	S-L		GO-014						
							NO_2, O_2, and either Ag or Ag_2O		PA-013	Kinetic studies showed that there was an induction time at lower temperatures (~ 1 hour at 450°C) which decreased with increasing temperature. At relatively high temperatures or beyond the induction period, the decomposition was first order. At 520°C, the activation energy was reported to be ~ 14 ± 2 kcal/mole.
						DTA was used from 50 to 744 at heating rate of 15°C/min. No product analysis			GO-014	
					(cont.)	(cont.)	(cont.)	(cont.)	(cont.)	(cont.)

COMPOUND	TRANSITIONS				DECOMPOSITION					DISCUSSION
	T(°C)	Type	ΔH(kcal/mole)	Ref.	T(°C)	Method/Comments	Products	Reactions	Ref.	
59. $AgNO_3$ (cont.)						was performed.				
					214	Fusion				
					305	Rapid bubbling occurred.				
					469	Rapid nitrous fumes were observed.				
						TGA was used.				
					444	$AgNO_3$ was reported to be stable up to this temperature, at which sudden evolution of nitrous vapors occurred.	Ag, "nitrous vapors", HNO_3 vapors.		DU-011	This decomposition temperature is in general agreement with most other studies (PA-013, GO-014). However Stern reports a much lower value.
					608	Formation of metallic silver.				
60. Zinc Nitrite										No evidence for the existence of this compound was found in the literature.
61. $Zn(NO_3)_2$					100	Stable up to this point.		$Zn(NO_3)_2 \rightleftarrows ZnO + 2NO_2 + \frac{1}{2}O_2$ (96)	ST-026	
					240	Slight decomposition.				
					>240	Decomposition becomes increasingly rapid.	ZnO, NO_2, O_2			
62. $Zn(NO_3)_2 \cdot 6H_2O$	36.1	S-L		RO-007		TGA was used to study the decomposition of this hydrated nitrate in air. The heating rate was 5.4°C/min.	ZnO	None given	WE-021	The gaseous decomposition product was assumed to be NO_2 since the reaction was carried out in a slow stream of air.
					40	Salt began to dehydrate.				
					160	Intermediate product, $Zn(NO_3)_2$				
					340	Constant weight, formation of ZnO.				
					(cont.)	(cont.)	(cont.)	(cont.)	(cont.)	(cont.)

COMPOUND	TRANSITIONS				DECOMPOSITION					DISCUSSION
	T(°C)	Type	ΔH(kcal/mole)	Ref.	T(°C)	Method/Comments	Products	Reactions	Ref.	
62. $Zn(NO_3)_2 \cdot 6H_2O$ (cont.)						DTA was used to study the behavior of this salt from 40 to 740. A heating rate of 15°C/min. was employed.	NO_2, HNO_3	None given.	GO-014	
					42	Hydrate dissolution.				
					281	Slight "nitrous fumes" (brown NO_2 and nitric acid).				
					332	Rapid "nitrous fumes".				
					470	Thermal reaction complete.				
					25-30 120-160 290-295	Thermal effects were reported at these temperatures from a TGA study.			SH-018	The abstract of this paper stated that the thermal effects recorded were due to dehydration, fusion, or decomposition. A comparison of these results with those above shows the first effect probably is hydrate dissolution, the second corresponds to dehydration (WE-021), and the third to nitrate decomposition (GO-014, WE-021).
63. $Cd(NO_3)_2$									PR-010	This compound slightly contaminated with the basic salt is reported to decompose slowly in air with evolution of nitrogen oxides and formation of a water-insoluble mass containing a mixture of basic salts.
64. $Cd(NO_3)_2 \cdot 2H_2O$						TGA study from 0 to 500°C.			PR-010	
					44	The dihydrate melts with partial loss of water.	H_2O			
					119	Dehydration complete	$Cd(NO_3)_2$			
					(cont.)	(cont.)	(cont.)	(cont.)	(cont.)	(cont.)

	TRANSITIONS				DECOMPOSITION					
COMPOUND	T(°C)	Type	ΔH(kcal/mole)	Ref.	T(°C)	Method/Comments	Products	Reactions	Ref.	DISCUSSION
64. $Cd(NO_3)_2 \cdot 2H_2O$ (cont.)					247	Endothermic effect due to nitrite decomposition and formation of basic salts.	Basic salts.			
					328,341	Decomposition of basic salts.				
					371.7	Formation of final product.	CdO			
65. $Cd(NO_3)_2$	360	S-L	4.3	ST-026	300	Rapid decomposition takes place above this temperature.	CdO, NO_2, O_2	$2Cd(NO_3)_2 \rightleftarrows 2CdO + 4NO_2 + O_2$ (97)	ST-026	The decomposition is reported to be reversible and to yield no intermediates.
									BA-040	The effect of 5 mole% addition of Ni, [illegible] Zn, and Ag nitrate [illegible] $Cd(NO_3)_2$ decom[illegible]ition was investigated. All additives were reported to have decreased the decomposition temperature from 360°C to 335-45°C and to have increased the rate of reaction. Note that 360°C was reported by Stern (ST-026) as the melting point.
66. $Cd(NO_3)_2 \cdot 4H_2O$	59.5	S-L	7.8	RO-007		TGA was used in this investigation. The heating rate was 5.4°C/min. and the reaction took place in a slow stream of air. The following temperatures of interest were reported:		None given	WE-021	The gaseous products were assumed to be NO_2 since the reaction took place in air.
					50	Salt began to lose water of hydration, followed by rapid weight loss.				
					220-280	Constant weight.	$Cd(NO_3)_2$			
					> 280	Nitrogen oxides evolved.				
					435	Oxide level	CdO			
					(cont.)	(cont.)	(cont.)	(cont.)	(cont.)	(cont.)

	TRANSITIONS				DECOMPOSITION					
COMPOUND	T(°C)	Type	ΔH(kcal/mole)	Ref.	T(°C)	Method/Comments	Products	Reactions	Ref.	DISCUSSION
66. $Cd(NO_3)_2 \cdot 4H_2O$ (cont.)						The method employed in this study was DTA. The standard employed was alumina and the heating rate was 15°C/min. Both thermograms and visual observations were reported.		None given	GO-014	
					66	Hydrate solution.				
					345	Slight "nitrous" fumes (brown NO_2)				
					379	Rapid "nitrous" fumes.				
					540	Decomposition complete.				
					30-50 110-200 350-80	This TGA study resulted in three thermal effects.			SH-018	The abstract of the paper did not specifically identify the thermal effects. It stated that all effects were due to either dehydration, fusion, or decomposition. If compared to the results above (WE-021, GO-014), it appears that the first effect is due to fusion of the nitrate in its water of crystallization The second effect corresponds to dehydration, and the last to nitrate decomposition.
67. $Al(NO_2)_3$										No evidence for the existence of this compound was found.
68. $Al(NO_3)_3$									ST-026	This compound has been prepared by vacuum sublimation of its adduct with N_2O_5. It condensed as a white powder at -78°C. None of its properties have been measured as yet.
69. $Al(NO_3)_3 \cdot 9H_2O$					150-450	Temperature range in the reaction chamber in which decomposi-	alumina HNO_3, H_2O, N_2O_5		AB-003	Time, temperature, and steam ratio were varied in this study to determine optimal conditions
					(cont.)	(cont.)	(cont.)	(cont.)	(cont.)	(cont.)

	TRANSITIONS				DECOMPOSITION					
COMPOUND	T(°C)	Type	ΔH(kcal/mole)	Ref.	T(°C)	Method/Comments	Products	Reactions	Ref.	DISCUSSION
69. $Al(NO_3)_3\cdot 9H_2O$ (cont.)						tion occurred in the presence of steam.				for nitrogen recovery in the form of HNO_3. It was found that in the presence of steam, N_2O_5 was formed which is easily converted to HNO_3.
						DTA was used.		$Al(NO_3)_3\cdot 9H_2O$	DR-002	This study was undertaken to determine the sequence of phase conversions during thermal decomposition in air. The dependence of the rates of these processes on temperature was also of interest. The following methods were employed: thermal analysis, high temperature X-ray diffraction, IR spectroscopy, optical crystallography, and others.
					70-400	Deep endotherm with 3 parts:		$\downarrow$ 70-100°		
					70-110	I. Dehydration to lower hydrate.	$Al(NO_3)_3\cdot 6H_2O$	$Al(NO_3)_3\cdot 6H_2O$		
					110-120	II. Removal of hygroscopic moisture.	H_2O	$\downarrow$ 160-180° $nAl_2O_3\cdot mN_2O_5\cdot pH_2O$		
					160-180	III. Decomposition to basic salts.		$\downarrow$ 200-400° Al_2O_3 amorph. (98)		
					>200	Formation of amorphous substance.				
					390	Completion of decomposition and formation of oxide.	Al_2O_3			
						$Al(NO_3)_3\cdot 9H_2O$ was held at a temperature of 150 for 5 to 10 hours until evolution of HNO_3 vapor ceased.	$Al_2(OH)_5NO_3$	$3Al(NO_3)_3\cdot 9H_2O \rightarrow Al_3(OH)_8NO_3 + 8HNO_{3(g)} + 19H_2O_{(g)}$ (99)	MA-042	The decomposition was halted at this temperature to determine the composition of the stable, intermediate basic nitrate.
					95	First appearance of HNO_3 vapors.	Spectrometric analysis of gaseous products showed traces of HNO_3.		KA-022	
					<120	Melting in its water of crystallization.				
					120-160	Simultaneous boiling of the melt and decomposition of the nitrate.				
					137	Maximum concentration (6.78%) HNO_3 vapors recorded at this temperature.				
					308-336	Unexplained endothermic effect.				
					(cont.)	(cont.)	(cont.)	(cont.)	(cont.)	(cont.)

	TRANSITIONS				DECOMPOSITION					
COMPOUND	T(°C)	Type	ΔH(kcal/mole)	Ref.	T(°C)	Method/Comments	Products	Reactions	Ref.	DISCUSSION
69. $Al(NO_3)_3\cdot 9H_2O$ (cont.)						TGA was used to study the decomposition in air with a heating rate of 5.4°C/min. The following temperatures of interest were reported:	No analysis of gaseous products.	None given.	WE-021	No evidence for the anhydrous nitrate or any other stable intermediate was found in this study.
					50	Slow loss of water.	H_2O			
					90	Weight loss became rapid.				
					460	Oxide level.	Al_2O_3			
70. Gallium Nitrite										No evidence for the existence of this compound was found.
71. $Ga(NO_3)_3$					40	Dehydration	$Ga(NO_3)_3$		ST-026	Stern reported that this compound was probably prepared by dehydration of the hydrate under vacuum at 40°C. A large fraction of the salt was reported to have been converted to Ga_2O_3 at 200°C.
					200	Formation of oxide	Ga_2O_3			
72. Indium Nitrite										No evidence for the existence of this compound was found.
73. $In(NO_3)_3$					90	Compound is stable at least up to this temperature.			ST-026	This nitrate was prepared at 90°C.
74. TlNO	169	S-S		ST-026						
	186	S-L								
75. $TlNO_3$	61.2	S-S	0.239	ST-026	266-340	Experimental range of vaporization study. In addition to decomposition, $TlNO_3$ was found to vaproize as the salt.	NO	$2TlNO_{3(c)} \rightarrow Tl_2O_{(c)} + 2NO_{2(g)} + \frac{1}{2}O_{2(g)}$ (100)	ST-026	Vapor pressure data for the range 490-612°K are reported.
	143	S-S	0.91							
	210	S-L	2.1							
	205	S-L	2.26	WE-021 ST-026 (Kleppa & Mc-Carthy)						
	(cont.)	(cont.)		(cont.)	(cont.)	(cont.)	(cont.)	(cont.)	(cont.)	(cont.)

	TRANSITIONS				DECOMPOSITION					
COMPOUND	T(°C)	Type	ΔH(kcal/mole)	Ref.	T(°C)	Method/Comments	Products	Reactions	Ref.	DISCUSSION
75. $TlNO_3$ (cont.)	75 143	S-S S-S		NE-003	50	Small amounts of absorbed water were lost.	$TlNO_3$, H_2O		WE-021	The study was done with TGA in a stream of air: The unknown species reported in the 460-505° range reportedly did not correspond to either Tl_2O or Tl_2O_3. Further weight loss beginning at 505°C indicates that the intermediate is either volatile or decomposes into volatile products.
					60	Anhydrous form.				
					265	Nitrogen oxides were evolved.				
					460-505	Intermediate level of unknown composition.				
					505-725	Continued weight loss until termination of experiment.				
76. Germanium Nitrite										No evidence for the existence of this compound has been found.
77. Germanium Nitrate										No evidence for the existence of this compound was found.
78. Tin Nitrite										No evidence for the existence of this compound has been found.
79. $Sn(NO_3)_4$	91	S-L		ST-026	98	Decomposition begins.	SnO_2		ST-026	No intermediate oxide-nitrate was found.
80. $Pb(NO_3)_2$						TGA was used with continuous removal of gaseous products. Decomposition products were analyzed using IR and UV spectroscopy. Gaseous products were also analyzed.		$3Pb(NO_3)_2 \rightleftarrows Pb(NO_2)_2 + 2PbO + 4NO$ (101)	PA-013	Patil was unable to identify the stable intermediate formed between 320 and 450. The stoichiometry indicated that the product was $Pb(NO_2)_2$, however the authors pointed out that the nitrite should be unstable at that temperature since it begins to decompose as low as 150. The fact that lead was found to undergo some oxidation (final product $PbO_{1.7}$) indicated that reaction (102) could have taken place: $Pb(NO_2)_2 + 2NO \rightleftarrows Pb(NO_3)_2 + 2NO_2$ (102) Reaction (102) would
					110-230	Weight loss.				
					230-300	Constant weight. Stoichiometry corresponded to 2PbO and $Pb(NO_2)_2$.	$Pb(NO_2)_2$, PbO, NO			
					300-320	Weight loss.				
					(cont.)	(cont.)	(cont.)	(cont.)	(cont.)	(cont.)

	TRANSITIONS				DECOMPOSITION					
COMPOUND	T(°C)	Type	ΔH(kcal/mole)	Ref.	T(°C)	Method/Comments	Products	Reactions	Ref.	DISCUSSION
80. $Pb(NO_3)_2$ (cont.)					320-450	Constant weight. Product not identified.				account for the presence of nitrite. Since product gases were removed the reaction would have to take place in the melt.
					450-500	Weight loss.	NO not evolved.			
					500	Constant weight. Product identified as $PbO_{1.7}$	$PbO_{1.7}$			
81. $Pb(NO_3)_2$						The decomposition was studied by measuring the total pressure and analyzing the solid phases. Product gases were continually removed.	Final Products: NO_2, O_2, PbO. Intermediates: $Pb(NO_3)_2 \cdot 2PbO$, $Pb(NO_3)_2 \cdot 5PbO$.	$6Pb(NO_3)_2 \rightleftarrows 2Pb(NO_3)_2 \cdot 2PbO + 8NO_2 + 2O_2$ (103a) $2Pb(NO_3)_2 \cdot 2PbO \rightleftarrows Pb(NO_3)_2 \cdot 5PbO + 2NO_2 + \frac{1}{2}O_2$ (103b) $Pb(NO_3)_2 \cdot 5PbO \rightleftarrows 6PbO + 2NO_2 + \frac{1}{2}O_2$ (103c) Overall: $6Pb(NO_3)_2 \rightleftarrows 6PbO + + 12NO_2 + 3O_2$ (103d) or, $Pb(NO_3)_2 \rightleftarrows PbO + 2NO_2 + \frac{1}{2}O_2$ (103e)	ST-026	Stern described the work of Neumann and Sonntag and the original article [Z. Elekt., 39, 799 (1933)] was not consulted. In contrast to Patil (PA-013) see below, Neumann and Sonntag found no oxidation of lead. Their identification of the basic nitrate intermediate which they formulated as $3PbO \cdot N_2O_5$ agrees with the stoichiometry found by Patil in the range 230-300 for nitrite decomposition. The product $6PbO \cdot N_2O_5$ or $Pb(NO_3)_2 \cdot 5PbO$, stable in the range from 352 to 462, might also be the unidentified stable intermediate found by Patil in the range 320 to 450.
					266-359	The product was $Pb(NO_3)_2 \cdot 2PbO$.				
					352-462	The product was $Pb(NO_3)_2 \cdot 5PbO$.				
					415-536	The product was PbO.				
						TGA was used with a stream of air to remove gaseous products. The heating rate was 5.4°C/min.	Final Product: PbO. Intermediate: $Pb(NO_3)_2 \cdot PbO$	None given.	WE-021	The intermediate found by Wendlandt did not have the same composition as those of Neumann and Sonntag. The final product was PbO, in agreement with Neumann but not with Patil.
					245	Beginning of slow weight loss.				
					370-435	Rapid weight loss and evolution of nitrogen oxides.				
					435	Break in the thermogram. Composition corresponded to $Pb_2O(NO_3)_2$ or $Pb(NO_3)_2 \cdot PbO$. Very limited stability.				
					(cont.)	(cont.)	(cont.)	(cont.)	(cont.)	(cont.)

COMPOSITION	TRANSITIONS T(°C)	Type	ΔH(kcal/mole)	Ref.	DECOMPOSITION T(°C)	Method/Comments	Products	Reactions	Ref.	DISCUSSION
81. $Pb(NO_3)_2$ (cont.)					435-575	Rapid decomposition.				
					575-	Constant weight. PbO was the product.				
						TGA was used with continuous removal of gaseous products. Solid products were analyzed by IR and UV spectroscopy.	Final product: $PbO_{1.4}$	None given	PA-013	Patil also investigated the decomposition of lead nitrate, but he did not publish details of the results. He did report that the final product had the composition $PbO_{1.4}$, indicating that some oxidation took place. He cited the work of Vratny and Gugliotta [J. Inorg. Nucl., 25, 1129 (1963)] in which it was reported that significant oxidation took place during $Pb(NO_3)_2$ decomposition. The results are clearly in disagreement.
					230- ?	Constant weight. Composition not reported.				
						No other details reported.				
82. Bismuth Nitrite										No evidence for the existence of this compound was found.
83. $Bi(NO_3)_3$						The reaction was studied on a thermobalance with a heating rate of 5°C/min.			LA-024	
					90	Decomposition begins.				
					100-250	Rate of decomposition at a maximum.				
					560	Oxide formed	Bi_2O_3			
84. $Bi(NO_3)_3 \cdot 5H_2O$					40	The nitrate melts in its water of crystallization; some HNO_3 is given off.	HNO_3, $BiONO_3$		LA-024	An intermediate oxynitrate was reported in this study. Note that the rate of reaction increases at 100°C for both the pentahydrate and the anhydrous nitrate (see above). The same oxide is observed as a final product at approximately the same temperature.
					100	Rate of decomposition becomes very fast at this point.				
					(cont.)	(cont.)	(cont.)	(cont.)	(cont.)	(cont.)

COMPOUND	TRANSITIONS T(°C)	Type	ΔH(kcal/mole)	Ref.	DECOMPOSITION T(°C)	Method/Comments	Products	Reactions	Ref.	DISCUSSION
84. $Bi(NO_3)_3 \cdot 5H_2O$ (cont.)					180	Reaction slows down.				
					600	Oxide level	Bi_2O_3			
					~49	Loses water of crystallization.			DU-011	The exact identity of the original substance was not given, but from comparison with $Bi(NO_3)_3 \cdot 5H_2O$ (LA-024), it appears to be the pentahydrate.
					49-600	Slow weight loss.				
					~600	Forms oxide.	Bi_2O_3			
85. $BiONO_3$					190	Stable up to this point.			LA-024	
					500-	Constant weight.	Bi_2O_3			
86. $BiONO_3 \cdot H_2O$						TGA was used in a stream of air at a heating rate of 54°C/minute.			WE-021	No stable anhydrous $BiONO_3$ intermediate was detected. Both this hydrate and its anhydrous form reached the oxide level within 5°C of each other in two separate experiments (LA-024, WE-021).
					50	Loss of water of hydration				
					505	Constant weight reached.	Bi_2O_3			
87. Zirconium Nitrite										No evidence of the formation of this compound was found.
88. $Zr(NO_3)_4$									ST-026	This compound has been prepared and is reported to be very hygroscopic.
89. $ZrO(NO_3)_2 \cdot 5H_2O$						TGA study at heating rate of 45°C/minute.	ZrO_2		WE-027	No stable intermediate was observed.
					575	Oxide formed.				
90. Molybdenum Nitrite										No evidence for the existence of this compound was found.
91. Molybdenum Nitrate										No evidence for the existence of this compound was found.
92. Tungsten Nitrite										No evidence for the existence of this compound was found.

	TRANSITIONS				DECOMPOSITION					
COMPOUND	T(°C)	Type	ΔH(kcal/mole)	Ref.	T(°C)	Method/Comments	Products	Reactions	Ref.	DISCUSSION
93. Tungsten Nitrate										No evidence for the existence of this compound was found.
94. Hafnium Nitrite										No evidence for the existence of this compound was found.
95. Hafnium Nitrate										No evidence for the existence of this compound was found.
96. Tantalum Nitrite										No evidence for the existence of this compound was found.
97. Tantalum Nitrate										No evidence for the existence of this compound was found.

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TECHNICAL NOTE 200-007-09

MATERIAL BALANCE CALCULATIONS FOR NO_x AQUEOUS SORPTION IN A PACKED TOWER

7 June 1971

Prepared by:

Terry B. Parsons

1.0 INTRODUCTION

This note described the calculations performed in making a material balance around a packed tower used for aqueous sorption of gaseous NO and NO_2. The system is shown in Figure 1.

Nitrogen oxides are present in several different forms. Some basis must therefore be chosen to describe the distribution of nitrogen among the various possible molecules. Chemical NO, C_{NO}, and chemical NO_2, C_{NO_2}, have been used previously and are defined for the gas phase in Equations 1 and 2 where n is number of moles.

$$C_{NO} = n_{NO} + n_{N_2O_3} + \tfrac{1}{2}n_{HNO_2} - \tfrac{1}{2}n_{HNO_3} \qquad (1)$$

$$C_{NO_2} = n_{NO_2} + 2n_{N_2O_4} + n_{N_2O_3} + \tfrac{1}{2}n_{HNO_2} + \tfrac{3}{2}n_{HNO_3} \qquad (2)$$

In the liquid phase most of the nitrogen oxides exist as nitrite and nitrate and the equations are written as in (3) and (4).

$$C_{NO} = \tfrac{1}{2}n_{NO_2^-} - \tfrac{1}{2}n_{NO_3^-} \qquad (3)$$

$$C_{NO_2} = \tfrac{1}{2}n_{NO_2^-} + \tfrac{3}{2}n_{NO_3^-} \qquad (4)$$

Chemical NO and NO_2 in the gas phase can be obtained from IR and UV analyses. Actually it is the molecules NO and NO_2 that are measured. But, at the measurement temperature NO and NO_2 are equal to chemical NO and NO_2 within less than 1%. Chemical

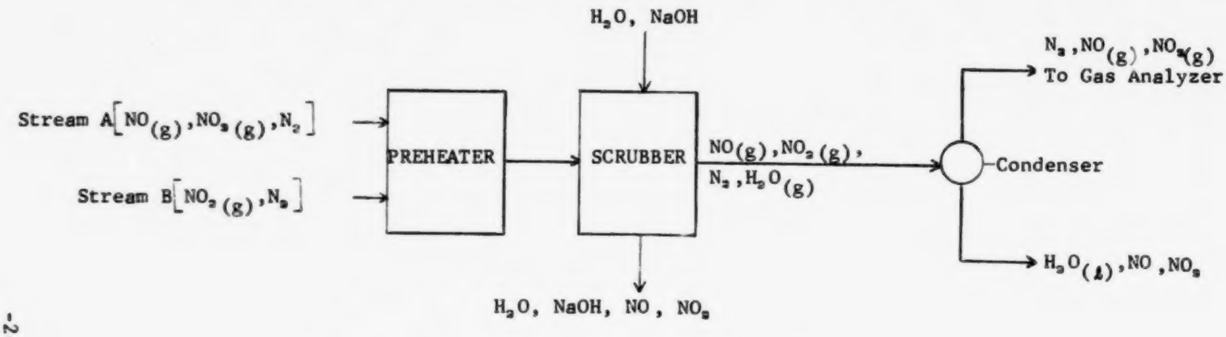
H_2O, NaOH
Stream A[$NO_{(g)}$, $NO_{2(g)}$, N_2]
Stream B[$NO_{2(g)}$, N_2]
PREHEATER
SCRUBBER
$NO(g)$, $NO_2(g)$, N_2, $H_2O_{(g)}$
Condenser
N_2, $NO_{(g)}$, $NO_{2(g)}$ To Gas Analyzer
$H_2O_{(l)}$, NO, NO_2
H_2O, NaOH, NO, NO_2

FIGURE 1

NO and NO_2 in the liquid phase are obtained by measuring nitrite and nitrate.

The material entering and leaving the scrubber is expressed in gram-moles of NO and NO_2 per minute. The number of moles per minute was calculated from measured concentrations and from flow rates obtained from corrected rotameter readings. The calculations are discussed in more detail in the following sections.

2.0 GAS ENTERING THE SCRUBBER

The gas flow rates were measured using rotameters calibrated with air at 77°F and 1 atm. However, nitrogen was used as the carrier gas in the actual experiments so a correction was needed for the molecular weight (density) difference. The calibration was carried out at a pressure of 1 atm or 29.9 inches mercury. The flow measurements were conducted with pressure differences of up to 6 inches of mercury gage so that a pressure correction was also necessary. The magnitude of the corrections was calculated by considering Brown's* equations for mass rate of flow of a fluid through a rotameter.

$$W = C_R A_o \left[\frac{2g\rho(\rho_f - \rho)V_f}{A_f(1 - A_o^2/A_1^2)}\right]^{\frac{1}{2}} \quad (1)$$

$$\approx C_R A_o \left[2g\rho\rho_f V_f/A_f\right]^{\frac{1}{2}} \quad (2)$$

$$= C_R^* A_o \rho^{\frac{1}{2}} \quad (3)$$

---

* Brown, G. G., et al., Unit Operations, p. 162, John Wiley and Sons, New York, (1952).

In Equations 1, 2, and 3 the following symbols have been used:

W = mass rate of flow per second

C_R = coefficient of discharge, a function of Reynold's number

A_o = annular area of the rotameter

g = acceleration due to gravity

ρ = gas density

V_f = volume of float

A_f = maximum cross sectional area of float

ρ_f = density of float

For an ideal gas:

$$\rho/M = n/V = P/RT \quad (4a)$$

or

$$\rho = PM/RT \quad (4b)$$

where M is the gram molecular weight.

Substituting (4b) into (3):

$$W = C_R^{\dagger} A_o (PM/RT)^{\frac{1}{2}} \quad (5)$$

We wish to express the rate of flow in terms of moles rather than mass, so (5) can be rewritten:

$$W/M = C_R^T A_0 \left(\frac{P}{MRT}\right)^{\frac{1}{2}} \qquad (6)$$

The factors for pressure corrections were calculated from Equation 7.

$$(P/29.9)^{\frac{1}{2}} \cong 1 + (\Delta P/2)/29.9 \qquad (7)$$

where P is the pressure at which experiments were conducted and ΔP is the pressure drop measured in inches of mercury.

The rotameter calibration curves were in units of standard cubic feet per hour. The factor for conversion to gram moles per minute, including the correction for the difference in molecular weights of air and nitrogen, is 2.04×10^{-3}. It was found that the maximum temperature correction would not exceed .007% so a temperature correction was not applied.

Gas entered the preheater in two separate streams, each having a slightly different flow rate. The flow rates were converted from units of standard cubic feet per hour to total moles per minute, so multiplication by the concentration of NO or NO_2 in each stream gave the rate of flow in moles chemical NO or NO_2 per minute. One entering stream contained both NO and NO_2 as shown by IR and UV analysis. The other entering stream was assumed to contain NO_2 only, however, the stream was not analyzed for NO. A summary of the calculations for gas entering the scrubber is given in Table I.

TABLE I
GAS ENTERING THE SCRUBBER

	Flow Rates $\hat{N}$ in total moles/minute		Concentrations in ppm				Entering	
			NO		NO_2			
RUN NO.	Stream A $\hat{N}_A$	Stream B $\hat{N}_B$	Stream A NO_A	Stream B NO_B	Stream A NO_{2A}	Stream B NO_{2B}	$\frac{\text{moles NO}}{\text{minute}} \times 10^6 = NO_A\hat{N}_A + NO_B\hat{N}_B$	$\frac{\text{moles } NO_2}{\text{minute}} \times 10^6 = NO_{2A}\hat{N}_A + NO_{2B}\hat{N}_B$
1	.2936	.2483	350	---	120	256	102.76	101.03
2	.3873	.3182	350	---	120	265	135.60	130.80
3	.4938	.3877	350	---	120	265	172.80	162.00

3.0 GAS LEAVING THE CONDENSER

The two entering streams were combined in the preheater before entering the scrubber, so the total gas flow leaving the scrubber was just the sum of the two entering rates. Again the concentrations were measured using IR and UV analysis. The gas stream leaving the scrubber, however, was saturated with water vapor which had to be removed since it interferes in the IR analysis. The water vapor was removed in a condenser in which some of the NO and NO_2 were also removed. The calculation of moles of NO and NO_2 removed per minute in the condenser is discussed in Section 5.0. The calculations for moles chemical NO and NO_2 leaving the condenser per minute are summarized in Table II.

4.0 LIQUID LEAVING THE SCRUBBER

The amount of NO and NO_2 leaving the scrubber in the scrubbing liquid was calculated by multiplying liquid flow rate in ml water per minute by the concentrations of nitrate and nitrite measured using wet chemical methods. The liquid flow was not varied in the three experiments. Nitrite and nitrate are related to chemical NO and NO_2 as discussed in Section 1.0. The calculations for chemical NO and NO_2 leaving in the scrubber liquid are summarized in Table III.

5.0 NO AND NO_2 LEAVING IN THE CONDENSATE

The amount of chemical NO and NO_2 leaving in the condensate in moles per minute was calculated by multiplying the number of ml water condensed per minute by the concentrations of nitrite and nitrate in the condensate. The condensation rate in ml H_2O per minute was calculated as follows:

TABLE II

GAS LEAVING THE CONDENSER

RUN NO.	Gas Flow $\left(\frac{\text{total moles}}{\text{minute}}\right)$ $N_{out} = \dot{N}_A + \dot{N}_B$	Concentration (ppm) NO	Concentration (ppm) NO_2	Material Leaving the Condenser $\frac{\text{moles NO}}{\text{minute}} \times 10^6 = \dot{N}_{out}NO$	Material Leaving the Condenser $\frac{\text{moles } NO_2}{\text{minute}} \times 10^6 = \dot{N}_{out}NO_2$
1	0.5419	180	97.5	97.54	52.84
2	0.7055	190	97.5	134.05	68.79
3	0.8815	210	97.5	185.12	85.95

TABLE III

LIQUID LEAVING SCRUBBER

RUN NO.	$\dot{W}$ = Liquid Flow (ml H_2O/minute)	Concentration (mg/ℓ) NO_2^-	Concentration (mg/ℓ) NO_3^-	Material Leaving in the Scrubbing Liquid (moles/minute x 10^6) $\dot{N}O_2^- = \dot{W}NO_2^-$	$\dot{N}O_3^- = \dot{W}NO_3^-$	$C_{NO} = \frac{\dot{N}O_2^- - \dot{N}O_3^-}{2}$	$C_{NO_2} = \frac{\dot{N}O_2^- + 3\dot{N}O_3^-}{2}$
1	710	4.00	1.70	61.74	19.47	21.14	60.08
2	710	4.15	1.80	64.05	20.61	21.72	62.95
3	710	4.58	2.05	70.69	23.48	23.61	70.56

$$\frac{\text{moles } H_2O \text{ condensed}}{\text{minute}} = \left(\frac{\text{moles } H_2O_{(g)}}{\text{minute}}\right)_{in} - \left(\frac{\text{moles } H_2O_{(g)}}{\text{minute}}\right)_{out} \quad (8)$$

$$\frac{\text{moles } H_2O_{(g)}}{\text{minute}} \cong \frac{\text{total moles gas}}{\text{minute}} \left(\frac{P^*_{H_2O}}{P_{N_2}}\right) \quad (9)$$

The total pressure is assumed to be closely approximated by $P_{N_2} + P^*_{H_2O}$, and it is assumed to be 1 atmosphere. $P^*_{H_2O}$ is the vapor pressure of water in mm of mercury at the temperature of interest. The temperature entering the condenser was 102°F and it was 60°F at the condenser outlet.

Substituting (9) into (8) gives:

$$\frac{\text{moles } H_2O_{(g)} \text{ condensed}}{\text{minute}} = \frac{\text{total moles gas}}{\text{minute}} \left(\frac{P^{102}_{H_2O}}{760-P^{102}_{H_2O}} - \frac{P^{60}_{H_2O}}{760-P^{60}_{H_2O}}\right) \quad (10)$$

$$= .056\ \dot{N}_{out} \quad (11)$$

where $\dot{N}_{out}$ is the gas flow leaving the scrubber. The condensation rate in ml H_2O/minute is obtained by multiplying by the molecular weight of water and assuming a solution density of 1g/ml. The only experiment for which the condensate was available for chemical analysis was Run 2. The calculations are summarized in Table IV.

TABLE IV

NO AND NO_2 LEAVING IN THE CONDENSER

RUN NO.	$W = \frac{\text{ml } H_2O \text{ Condensed}}{\text{minute}}$ $= (.056)(18)(\dot{N}_{out})$	Concentration (mg/ℓ)		Material Leaving in the Condensate $\left(\frac{\text{moles}}{\text{minute}} \times 10^6\right)$			
		NO_2^-	NO_3^-	$\dot{N}O_2^- = \frac{\dot{W}NO_2^-}{46}$	$\dot{N}O_3^- = \frac{\dot{W}NO_3^-}{62}$	$C_{NO} = \frac{\dot{N}O_2^- - \dot{N}O_3^-}{2}$	$C_{NO_2} = \frac{\dot{N}O_2^- + 3\dot{N}O_3^-}{2}$
1	0.5454						
2	0.7111	1.5	558.0	.0232	6.40	-3.19	9.61
3	0.8892						

6.0 SUMMARY

The results of the calculations discussed in Sections 2 through 5 are summarized in Table V. The chemical NO and NO_2 entering the scrubber should equal the sum of (1) chemical NO and NO_2 leaving the condenser, (2) chemical NO and NO_2 in the condensate, and (3) chemical NO and NO_2 in the scrubber liquid.

TABLE V
MATERIAL BALANCE SUMMARY

	Gas In (mole/min x 10^6)	Gas Out of Condenser	+	Scrubber Liquid Out (mole/min x 10^6)	+	Liquid Condensed	=	
Run 1 NO	102.76	97.54	+	21.14	+	?	=	118.68
NO_2	101.03	52.84	+	60.08	+	?	=	112.92
Run 2 NO	135.6	134.05	+	21.72	+	(-3.2)	=	152.57
NO_2	130.8	68.79	+	62.95	+	9	=	140.74
Run 3 NO	172.8	185.12	+	23.61	+	?	=	208.73
NO_2	162.0	85.95	+	70.56	+	?	=	156.51

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TECHNICAL NOTE 200-007-11

Selected Values for Equilibrium Constants Used in the Aqueous Equilibrium Formulation

10 September 1971

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1.0 INTRODUCTION AND BACKGROUND

In order to analyze process performance and design equipment for aqueous alkaline sorption processes it is necessary to develop a mathematical description of vapor-liquid, ionic, and liquid-solid equilibria which take place in the process. Radian has developed a vapor-liquid-solid formulation which calculates the equilibrium distribution among the various gaseous, aqueous, and crystalline species present in aqueous alkaline scrubbing processes. Part of the data required for this formulation are the values of thermodynamic equilibrium constants and activity coefficients at varying temperatures for the reactions and species of interest. The model was originally developed to describe limestone wet scrubbing processes for SO_2 removal. In order to extend the model to describe alkaline scrubbing processes for NO_x removal, equilibrium constants for the following reactions had to be added:

$$HNO_{3(g)} \rightleftarrows HNO_{3(\ell)} \qquad (1a)$$

$$HNO_{3(\ell)} \rightleftarrows H^+ + NO_3^- \qquad (1b)$$

$$HNO_{2(g)} \rightleftarrows HNO_{2(\ell)} \qquad (2a)$$

$$HNO_{2(\ell)} \rightleftarrows H^+ + NO_2^- \qquad (2b)$$

$$NO_{(g)} \rightleftarrows NO_{(\ell)} \qquad (3)$$

In addition, activity coefficients for the species $HNO_{2(\ell)}$, $HNO_{3(\ell)}$, NO_2^-, NO_3^-, and $NO_{(\ell)}$ were needed. This Technical Note documents the selection of equilibrium constants and activity coefficients from the literature for addition to the aqueous ionic equilibrium formulation.

2.0 ACTIVITY COEFFICIENTS

In the equilibrium formulation presently in use, equilibrium constants are defined in terms of activities (fugacities) of the reactants and products. The activities are the product of a molality and an activity coefficient. The activity coefficients, γ_i, are correlated as a function of ionic strength. The correlation form is the equation given in equation (4), where A and B are constants determined by the dielectric constant of the solvent, I is the ionic strength and Z_i the ionic charge for the $i^{\underline{th}}$ species.

$$\log \gamma_i = AZ_i^2 \left[\frac{-I^{\frac{1}{2}}}{1+B\mathring{a}_i I^{\frac{1}{2}}} + b_i I\right] + U_i I \qquad (4)$$

The parameters $\mathring{a}_i$, b_i, and U_i are characteristic of the ionic or uncharged species. For ionic species U_i is zero, and for uncharged species Z_i and b_i are zero. The values for $\mathring{a}_i$ and b_i were chosen so as to obtain a curve of $\log \gamma_i$ vs. I that closely agreed with those published by Garrels (GA-003), Klotz (KL-001), or Davies (DA-001) for the different ionic species of interest. For all uncharged aqueous species, U_i was chosen to be 0.076 from Garrels' value for H_2CO_3. Nitrate and hydrogen ion activity coefficient parameters were previously selected for the limestone based process description. For the alkaline scrubbing model, therefore, activity coefficient parameters for NO_2^-, $HNO_{2(\ell)}$, and $HNO_{3(\ell)}$ remained to be specified. The nitrate ion parameters were used to calculate nitrite ion activity coefficients. The value $U_i = .076$ was used for the uncharged species $HNO_{2(\ell)}$ and $HNO_{3(\ell)}$.

It should be pointed out that some mean ionic activity coefficient data for alkali metal nitrites exist

(RA-026, CH-041) which could be correlated using an extension of the mean salt method developed by Radian to obtain nitrite ion activity coefficient parameters (see Technical Note 200-403-22). In addition, Davis and deBruin (DA-012) critically evaluated all the data published concerning HNO_3 and calculated a consistent set of activity coefficients. Finally, Schmid and Krenmayr (SC-015) have investigated the activity coefficient of HNO_3 as a function of ionic strength for the equilibrium $HNO_{3(\ell)} \rightleftarrows N_2O_{3(\ell)} + H_2O$.

Radian has proposed further work to update the aqueous equilibrium model and increase its accuracy by including data such as those described above. The rather detailed process of data analysis required (see Technical Note 200-403-22) as well as the application of the equilibrium model to process design are, however, beyond the scope of Contract EHSD 71-5.

3.0 EQUILIBRIUM CONSTANTS

Publications reporting experimental measurements of the equilibrium constants of interest were found by consulting the compilation of Sillén, Stability Constants of Metal-Ion Complexes (SI-001). This compilation covered the literature up to 1960 and did not include data for vapor-liquid equilibrium constants such as those needed for reactions (1a) and (2a). Chemical Abstracts was also used to obtain these data and to obtain information published after 1960.

The literature had to be evaluated to insure that, if possible, constants were selected which were based on (1) data extrapolated to infinite dilution (I=0) and (2) activities rather than molalities. Data giving the temperature dependence of equilibrium constants were also necessary.

The following paragraphs describe how each of the equilibrium constants were selected or re-calculated for use in the equilibrium model.

3.1 Nitric Acid Dissociation Constant

Five references were consulted in selecting a value for the dissociation constant and temperature dependence of the constant for nitric acid. Hood and Reilly (HO-014) used proton magnetic resonance to measure the degree of dissociation, α, with some assumptions made concerning the proton shift of the undissociated acid. The equilibrium constant was calculated from determinations of α at 0, 25, and 70°C, using equation (5), a form of the Ostwald Dilution Law. γ_u is the activity coefficient of undissociated HNO_3, a is the activity, and C_s is the stoichiometric molar HNO_3 concentration.

$$K\ \gamma_u = \frac{a_{H^+} a_{NO_3^-}}{C_s(1-\alpha)} \qquad (5)$$

Log $K\gamma_u$ was extrapolated to obtain K at infinite dilution. Activity coefficients for 25°C had to be used to calculate activities at 0 and 70°C. The authors found ΔH_{298} for the dissociation reaction to be -3.3 kcal/mole from a plot of log K vs. $\frac{1}{T}$. Their K values are given in Table I. The values in parentheses resulted from calculating the proton shift for undissociated HNO_3 by assuming the degree of dissociation at 50 mole % HNO_3 is zero. If the proton shift is obtained using other data for α published by Krawetz (KR-012), the higher K values (not in parentheses) result.

TABLE I

Values of K_{diss} for HNO_3 Found by Hood and Reilly (HO-014) and Krawetz (KR-012)

T(°C)	K (HO-014)		K (KR-012)
0	48	(40)	45
25	27.5	(25)	23.5
50			17.5
70	15	(12.5)	

Krawetz (KR-012) used the same method as Hood and Reilly, except he used Raman spectra to determine the degree of dissociation. His values for the equilibrium constant are also given in Table I above.

Högfeldt (HO-015) considered the suggestion that the complexes $HNO_3(H_2O)_3$ and $HNO_3(H_2O)$, are formed between water and undissociated nitric acid. He represented the equilibria using (6) and (7).

$$H^+ + NO_3^- + iH_2O \rightleftarrows HNO_3(H_2O)_i \qquad (6)$$

$$a_{HNO_3(H_2O)_i} = K_{1,i}\, a_{H^+} a_{NO_3^-} a_{H_2O}^i \qquad (7)$$

Högfeldt assumed that measurements to determine degree of dissociation such as those carried out by Krawetz (KR-012) and Hood and Reilly (HO-014) could not distinguish between

undissociated HNO_3 and its complexes with water molecules. Therefore the quantity $C(1-\alpha)$ referred to the sum of molarities of undissociated HNO_3 and the complexes $HNO_3(H_2O)_i$. He further assumed that the activity coefficients of the water complexes were 1. Equations (8) and (9) followed.

$$C(1-\alpha) = \sum_i K_{1,i} a_{H^+} a_{NO_3^-} a_{H_2O}^i \qquad (8)$$

$$\frac{C(1-\alpha)}{a_{H^+} a_{NO_3^-}} = \sum_i K_{1,i} a_{H_2O}^i \qquad (9)$$

In a range where one i was predominant:

$$\log \left[\frac{C(1-\alpha)}{a_{H^+} a_{NO_3^-}}\right] = \log K_{1,i} + i \log a_{H_2O} \qquad (10)$$

Högfeldt pointed out that a plot of $\log \left[\frac{C(1-\alpha)}{a_{H^+} a_{NO_3^-}}\right]$ vs. $\log a_{H_2O}$ would show the values of i for a system. Further he claimed that a horizontal line would result for the range where i=0 and the complex $HNO_3(H_2O)_0$ is predominant. The asymptote would then give the value of $\log K_{1,0} = \log \left[\frac{C(1-\alpha)}{a_{H^+} a_{NO_3^-}}\right]$. Using previously published data for a_{H^+}, $a_{NO_3^-}$ and a_{H_2O} and Krawetz' data for $C(1-\alpha)$, Högfeldt determined $K_{1,0}$ or pK_{diss} to be -3.78. This results in a dissociation constant at 25°C of 6026 compared to a value of 23.5 (pK=-1.38) found by Krawetz. Högfeldt pointed out that the indicator 2,4-dichloro-6-nitroaniline acts as a base towards HNO_3. Therefore, the indicator should have a pK value greater than HNO_3 or HNO_3 should have a pK value smaller than the indicator, which has a pK value of -3.3.

Davis and deBruin (DA-012) measured the partial pressures of HNO_3 over 2-16M solutions and calculated a set of mean ionic and molecular activity coefficients which were consistent with some previously published data for higher concentrations. He used the data of Krawetz (KR-012) and Hood and Reilly (HO-014) for α. Using these coefficients, the dissociation constant was calculated according to equation (11)

$$K = \frac{\left(Y_s C_s\right)^2}{Y_u C_s (1-\alpha)} \qquad (11)$$

where $\left(Y_s C_s\right)^2 = \left(Y_\pm C_\pm\right)^2$ and Y is the activity coefficient and C the molality. The molality of stoichiometric HNO_3, C_s, is defined in equation (12) where u stands for undissociated.

$$C_s = C_u + C_\pm \qquad (12)$$

The value obtained by Davis and deBruin for K at 25°C was 18.8 ± 2.3. The data for α were edited to obtain this value and the authors pointed out the need for more accurate data.

Helgeson (HE-001) gave a theoretical treatment of a method of estimation of the temperature dependence of log K for dissociation reactions. The method is based on equation (13) which describes the free energy of the dissociation reaction.

$$\Delta F_r^\circ(T) = \Delta H_r^\circ(T_r) - T_r \Delta S_r^\circ(T_r) - \int_{T_r}^{T} \Delta S_r^\circ(T)\, dT \qquad (13)$$

$\Delta H_r^\circ(T_r)$ and $\Delta S_r^\circ(T_r)$ are the enthalpy and entropy of the dissociation reaction at the reference temperature, T_r, which is 298.15°K. Helgeson separated the variable $\Delta S_r^\circ(T)$ into a contribution due to electrostatic interaction, $\Delta S_e^\circ(T_r)$, and a contribution due to nonelectrostatic interaction, $\Delta S_n^\circ(T_r)$. The electrostatic entropy contribution was described as a function of temperature using the Born or Bjerrum expression for the linear relationship between the free energy of dissociation and the dielectric constant of the solvent. The nonelectrostatic entropy contribution was described as a function of temperature using equation (14)

$$\Delta S_n^\circ(T) = \Delta S_n^\circ(T_r) + \int_{T_r}^{T} \frac{\Delta Cp_n^\circ(T)}{T}\, dT \qquad (14)$$

In equation (14) the nonelectrostatic contribution to the heat capacity of dissociation $\Delta Cp_n^\circ(T)$ is defined by (15).

$$\Delta C_{pn^\circ}(T) = \alpha + \beta T + \lambda T^2 \qquad (15)$$

The coefficients α and β and the factor $\Delta S_e^\circ(T_r)$ were obtained by least squares fits of reported data. The λ coefficient was ignored.

Helgeson applied the method to many dissociation reactions. For the case of nitric acid, he used the data of Krawetz and Hood and Reilly as well as that of Noyes (NO-011) and Young et al (YO-007). He felt it was necessary to edit the data and exclude one of the high temperature points based on a personal communication that the nitrate ion disproportionates above 250°C. For the case of nitric acid $\Delta H_r^\circ(T_r)$ and $\Delta S_r^\circ(T_r)$ were also obtained by a least squares fit of the data. The value obtained by Helgeson for $\Delta H_r^\circ(T_r)$, -4,100 cal/mole, was the same as that obtained by Young (YO-007), using the data of Noyes (NO-011) and Krawetz (KR-012). Hood and Reilly, however, obtained a value of -3,300 cal/mole. Helgeson concluded that more high temperature data are required to determine log K(T) and $\Delta H_r^\circ(T_r)$.

In a compilation of ionization constants published in the same year as the theoretical work of Helgeson (HE-001), Barnes, Helgeson, and Ellis (BA-050) gave equation (16) for the temperature dependence of log K for nitric acid dissociation up to 300°C.

$$\log K = 6.557 - 320.88 \left(\frac{1}{T}\right) - 0.01359T \qquad (16)$$

This equation was based on the data of Young (YO-007) and Hood, Reilly and Redlich (HO-038). It gives a value of log K = 1.43 at 25°C. This value was used by Radian in the equilibrium formulation.

3.2 Nitrous Acid Dissociation Constant

The work of Klemenc and Hayek (KL-007), Vassian and Eberhardt (VA-011) and Lumme and Tummavuori (LU-005, TU-007) was reviewed in order to select an equilibrium constant for nitrous acid dissociation.

Klemenc and Hayek measured the conductivities of solutions of H_2SO_4 and $Ba(NO_2)_2$ at 0 and 12.5°C. In order to calculate the dissociation constant of HNO_2, the nitrite conductivity at infinite dilution was also needed. It was determined by measuring conductivities of KNO_2 solutions of varying concentrations and assuming KNO_2 is completely dissociated. Published transport numbers of H^+ and K^+ were used to calculate their conductivities at infinite dilutions. The data were used in (17) to calculate the dissociation constant.

$$K_\lambda = \frac{[H^+][NO_2^-]}{[HNO_2]} = \frac{C\ \lambda_{meas}^2}{\lambda_o(\lambda_o - \lambda_{meas})} \qquad (17)$$

In (17), C is the concentration in moles/ℓ, λ_o is the conductivity of HNO_2 at infinite dilution, which is the sum of conductivities of H^+ and NO_2^-, and λ_{meas} is the measured conductivity. The units of K_λ were moles/liter. The activity coefficients for each of the species were not taken into account. The results are given in Table II. The authors calculated a heat of dissociation of 4,480 cal but they did not specify the temperature or the method of calculation.

TABLE II

Results of Klemenc and Hayek (KL-007) for the Dissociation Constant of HNO_2

T°C	K(moles/ℓ)
0.	$3.2 \pm 0.3 \times 10^{-4}$
12.5	$4.6 \pm 0.4 \times 10^{-4}$
30.	$6.0 \pm 0.6 \times 10^{-4}$

During investigation of complex formation between cadmium and nitrite ions, it was necessary for Vassian and Eberhardt (VA-011) to take into account the dissociation constant for nitrous acid. They used a solution of .0226F KNO_2 adjusted to ionic strength 1.0 and .07 and pH 3.25. They measured C_{HNO_2} spectrophotometrically at 358 mμ which is one of the wavelengths of maximum absorption of HNO_2 (WA-015). Their results are given in Table III. Note that these investigators also ignored the activity coefficients of NO_2^- and HNO_2.

TABLE III

Results of Vassian and Eberhardt (VA-011) at 25°C for the Dissociation Constant of HNO_2

I	K (moles/ℓ)
.07	15.5×10^{-4}
1.0	15.9×10^{-4}

Lumme and Tummavuori (LU-005, TU-007) measured the dissociation constant of HNO_2 by performing potentiometric titrations at 15, 20, 25 and 35°C in solutions of sodium nitrite, nitrate, and perchlorate at varying ionic strengths. Their values were extrapolated to zero ionic strength using equation (18),

$$pK = pK_o + \frac{(-1.023)I^{\frac{1}{2}}}{1 + aI^{\frac{1}{2}}} + BI \qquad (18)$$

which in effect takes into account the activity coefficients since it is of the same form as semi-empirical correlations of log γ vs. I. The results, given in Table IV, were used in the equilibrium model.

TABLE IV

Nitrous Acid Dissociation Constant of Lumme and Tummavuori (LU-005, TU-007)

t°C	K
15	5.97×10^{-4}
25	7.24×10^{-4}
35	7.94×10^{-4}

The temperature dependence was also calculated and is given in (19). The data are valid up to 38°C.

$$\log K = -5.8554 \times 10^{3} \left(\frac{1}{T}\right) - 60.571 \times 10^{-3} T + 34.558 \qquad (19)$$

3.2 Vapor-Liquid Equilibrium Constant for Nitrous Acid

The only data found for the nitrous acid vapor-liquid equilibrium were published in 1929 by Abel and Neusser (AB-006).

The authors carefully conducted numerous equilibrium experiments in which they measured concentrations in both the gas phase and the aqueous phase. From the aqueous phase measurements, they provided sufficient data for calculating the activities of $HNO_{2(\ell)}$, H^+, and NO_2^-, since the dissociation constant of $HNO_{2(\ell)}$ is known. Since activity coefficients for these species were unknown at the time, Abel and Neusser's equilibrium constant was reported in concentration units.

The gas phase data were reported in units of concentration of nitrogen +3, which includes both $HNO_{2(g)}$ and $N_2O_{3(g)}$. Therefore a correction had to be made for the amount of $N_2O_{3(g)}$ present. After some recalculations, it was therefore possible to determine $K_1 = a_{HNO_{2(\ell)}}/a_{HNO_{2(g)}}$, the vapor liquid equilibrium constant, from the data of Abel and Neusser.

Abel and Neusser used a solution of KNO_2 and HNO_3 under 1 atm NO which was bubbled through the closed, constant temperature system to suppress the decomposition of nitrous acid according to reaction (20).

$$3HNO_2 \rightleftarrows H^+ + NO_3^- + 2NO + H_2O \qquad (20)$$

[Equation (20) is simply the sum of two times (21) plus two times (22) plus (23) plus (24)].

$$2HNO_2 \rightleftarrows N_2O_3 + H_2O \qquad (21)$$

$$N_2O_3 \rightleftarrows NO + NO_2 \qquad (22)$$

$$2NO_2 \rightleftarrows N_2O_4 \qquad (23)$$

$$N_2O_4 + H_2O \rightleftarrows HNO_2 + HNO_3 \qquad (24)$$

After allowing two days for the system to reach equilibrium, they measured (1) NO_2^- content in the reaction vessel using permanganate titration and back titration with oxalic acid and (2) the hydrogen ion concentration. The gas in equilibrium with the aqueous phase was absorbed in concentrated sulfuric acid. At the conclusion of the experiments nitrogen was bubbled through the gas absorption flask to drive off the "strongly held" dissolved NO which had a solubility of 46.9 mg/ℓ. The

nitrosylsulfuric acid formed by reaction of the absorbed +3 nitrogen with H_2SO_4 was titrated with permanganate.

Abel and Neusser's calculations did not take into account activity coefficients of the species of interest or equilibrium constants for the possible aqueous phase reactions. In addition, they did not correct for the equilibrium concentration of N_2O_3 in the vapor due to equation 21. Fortunately the authors published their experimental findings in detail and it was possible to recalculate the vapor-liquid equilibrium constant using the Radian aqueous equilibrium model. The aqueous equilibria of importance for the system are given in (25) through (28).

$$HNO_{3(\ell)} \rightleftarrows H^+ + NO_3^- \qquad (25)$$

$$HNO_{2(\ell)} \rightleftarrows H^+ + NO_2^- \qquad (26)$$

$$KNO_{2(\ell)} \rightleftarrows K^+ + NO_2^- \qquad (27)$$

$$KNO_{3(\ell)} \rightleftarrows K^+ + NO_3^- \qquad (28)$$

When the aqueous model was originally programmed and the equilibrium constants were selected some simplifications were made (LO-007, p.80). It was anticipated that in limestone wet scrubbing processes, the amounts of sodium and potassium would not be accurately known. Further, it was recognized that the complexes of sodium and potassium are "relatively weak and of the same order of magnitude". Some examples are given in Table V.

TABLE V

Dissociation Constants (SI-001) for Complexes of Sodium and Potassium

Reaction	Log K
$NaSO_4^- \rightleftarrows Na^+ + SO_4^=$	-.72
$KSO_4^- \rightleftarrows K^+ + SO_4^=$	-.96
$NaNO_3 \rightleftarrows Na^+ + NO_3^-$	.4 ± .1
$KNO_3 \rightleftarrows K^+ + NO_3^-$	.23 ± .03

Therefore, there was no provision made for calculations involving potassium. Instead, the constants for sodium were used and any potassium present was treated as the equivalent amount of sodium.

The data of Abel and Neusser were recalculated in the following manner. The measured molalities of NO_2^-, NO_3^- and K^+ were input to the equilibrium model and the ionic strength and activities of $HNO_{2(\ell)}$, H^+, and NO_2^- were calculated. It was assumed that KNO_2 is completely dissociated. The authors conducted experiments at ionic strengths of .2, .65, .7, .95, 1.25, 1.45, 2.5 and 3.5. Only the data taken at ionic strengths of 1.45 and below were used in Radian calculations (data from Abel and Neusser's Tables 1 through 6). The data were taken from columns 5, 7, 8, and 9 of the Tables. About 40 data points were used. The results are given in Table VI.

TABLE VI

Results of Calculations
Using the Data of Abel and Neusser (AB-006)
in the Radian Aqueous Equilibrium Model

163

RUN 112

```
29 JUN 71    11:11:52.263                                                   TEMPERATURE    25.000  DEG. C
                                        INPUT MOLES

 SO2  =0.00000
 CO2  =0.00000
 SO3  =0.00000        N2O5 =1.00000-01     CAO  =0.00000       MGO  =0.00000
 NA2O =7.50000-02     HCL  =0.00000        H2O  =5.57448+01    N2O3 =6.38000-02

                                   AQUEOUS SOLUTION EQUILIBRIA

             COMPONENT         MOLALITY            ACTIVITY       ACTIVITY COEFFICIENT
             H2O                                                        9.934-01
             H+                6.116-02            5.081-02             8.307-01
             OH-               2.659-13            1.980-13             7.447-01
             NO3-              1.947-01            1.236-01             6.348-01
             NA+               1.449-01            1.095-01             7.558-01
             NAOH              5.636-15            5.837-15             1.036+00
             NANO3             5.203-03            5.389-03             1.036+00
             HNO3              2.366-04            2.450-04             1.036+00
             NO2-              1.137-02            7.215-03             6.348-01
             HNO2              4.890-01            5.064-01             1.036+00

                                   MOLECULAR WATER = 9.99344-01 KGS.

               PH =       1.294          IONIC STRENGTH = 2.00375-01            RES. E.N. =  -6.665-10
```

RUN 113

```
29 JUN 71    11:11:53.749                                                   TEMPERATURE    25.000  DEG. C
                                        INPUT MOLES

 SO2  =0.00000
 CO2  =0.00000
 SO3  =0.00000        N2O5 =1.00000-01     CAO  =0.00000       MGO  =0.00000
 NA2O =7.50000-02     HCL  =0.00000        H2O  =5.57392+01    N2O3 =5.62500-02

                                   AQUEOUS SOLUTION EQUILIBRIA

             COMPONENT         MOLALITY            ACTIVITY       ACTIVITY COEFFICIENT
             H2O                                                        9.934-01
             H+                6.117-02            5.081-02             8.307-01
             OH-               2.659-13            1.980-13             7.447-01
             NO3-              1.947-01            1.236-01             6.348-01
             NA+               1.449-01            1.095-01             7.558-01
             NAOH              5.636-16            5.837-15             1.036+00
             NANO3             5.204-03            5.390-03             1.036+00
             HNO3              2.366-04            2.450-04             1.036+00
             NO2-              1.137-02            7.215-03             6.348-01
             HNO2              4.890-01            5.065-01             1.036+00

                                   MOLECULAR WATER = 9.99244-01 KGS.

               PH =       1.294          IONIC STRENGTH = 2.00394-01            RES. E.N. =  -1.700-10
```

RUN 105

```
29 JUN 71     11:11:59.132                                                    TEMPERATURE     25.000  DEG. C
                                              INPUT MOLES

 SO2   =0.00000
 CO2   =0.00000
 SO3   =0.00000       N2O5 =1.00000-01     CAO   =0,00000       MGO   =0.00000
 NA2O  =3,95000-02    HCL   =0.00000       H2O   =5,56898+01    N2O3  =4.43000-02

                                        AQUEOUS SOLUTION EQUILIBRIA

                COMPONENT          MOLALITY              ACTIVITY        ACTIVITY COEFFICIENT
                H2O                                                            9.934-01
                H+                 1.264-01              1.050-01              8.307-01
                OH-                1.287-13              9.587-14              7.448-01
                NO3-               1.972-01              1.252-01              6.351-01
                NA+                7.640-02              5.775-02              7.559-01
                NAOH               1.439-15              1.490-15              1.036+00
                NANO3              2.780-03              2.879-03              1.036+00
                HNO3               4.952-04              5.128-04              1.036+00
                NO2-               5.573-03              3.540-03              6.351-01
                HNO2               4.956-01              5.132-01              1.036+00

                                     MOLECULAR WATER = 9,97713-01 KGS.

                 PH =        .979           IONIC STRENGTH = 1.99970-01             RES. E.N. =   -3.505-11
```

RUN 103

```
29 JUN 71     11:11:55.096                                                    TEMPERATURE     25.000  DEG. C
                                              INPUT MOLES

 SO2   =0.00000
 CO2   =0.00000
 SO3   =0.00000       N2O5 =1.00000-01     CAO   =0,00000       MGO   =0.00000
 NA2O  =3.95000-02    HCL   =0.00000       H2O   =5,56870+01    N2O3  =4.15000-02

                                        AQUEOUS SOLUTION EQUILIBRIA

                COMPONENT          MOLALITY              ACTIVITY        ACTIVITY COEFFICIENT
                H2O                                                            9.934-01
                H+                 1.264-01              1.050-01              8.307-01
                OH-                1.287-13              9.586-14              7.448-01
                NO3-               1.972-01              1.252-01              6.351-01
                NA+                7.640-02              5.775-02              7.559-01
                NAOH               1.439-15              1.490-15              1.036+00
                NANO3              2.780-03              2.879-03              1.036+00
                HNO3               4.952-04              5.128-04              1.036+00
                NO2-               5.573-03              3.540-03              6.351-01
                HNO2               4.956-0               5.132-01              1.036+00

                                     MOLECULAR WATER = 9,97663-01 KGS.

                 PH =        .979           IONIC STRENGTH = 1.99980-01             RES. E.N. =   -3.619-11
```

```
                                              RUN 102
03 AUG 71    11:09:47.205                                              TEMPERATURE    25.000  DEG. C
                                       INPUT MOLES

 SO2  =0,00000
 CO2  =0.00000
 SO3  =0,00000       N2O5 =1.00000-01    CAO  =0,00000      MGO  =0.00000
 NA2O =3.95000-02    HCL  =0.00000       H2O  =5.56827+01   N2O3 =3.72000-02

                                  AQUEOUS SOLUTION EQUILIBRIA

          COMPONENT           MOLALITY             ACTIVITY        ACTIVITY COEFFICIENT
          H2O                                                            9.934-01
          H+                  1.264-01             1.050-01              8.307-01
          OH-                 1.287-13             9.585-14              7.448-01
          NO3-                1.972-01             1.252-01              6.351-01
          NA+                 7.641-02             5.776-02              7.559-01
          NAOH                1.439-15             1.490-15              1.036+00
          NANO3               2.781-03             2.860-03              1.036+00
          HNO3                4.953-04             5.129-04              1.036+00
          NO2-                5.574-03             3.540-03              6.351-01
          HNO2                4.956-01             5.133-01              1.036+00

                                  MOLECULAR WATER = 9.97585-01 KGS.

           PH =         .979          IONIC STRENGTH = 1.99995-01          RES. E.N. =  -1.506-09
```

```
                                              RUN 107
03 AUG 71    11:09:48.634                                              TEMPERATURE    25.000  DEG. C
                                       INPUT MOLES

 SO2  =0,00000
 CO2  =0,00000
 SO3  =0.00000       N2O5 =1.00000-01    CAO  =0.00000      MGO  =0.00000
 NA2O =9,80000-02    HCL  =0,00000       H2O  =5.57228+01   N2O3 =1.88000-02

                                  AQUEOUS SOLUTION EQUILIBRIA

          COMPONENT           MOLALITY             ACTIVITY        ACTIVITY COEFFICIENT
          H2O                                                            9.952-01
          H+                  2.811-02             2.336-02              8.312-01
          OH-                 5.791-13             4.306-13              7.437-01
          NO3-                1.933-01             1.221-01              6.316-01
          NA+                 1.894-01             1.429-01              7.546-01
          NAOH                1.598-14             1.657-14              1.037+00
          NANO3               6.703-03             6.948-03              1.037+00
          HNO3                1.074-04             1.113-04              1.037+00
          NO2-                2.421-02             1.529-02              6.316-01
          HNO2                4.761-01             4.935-01              1.037+00

                                  MOLECULAR WATER = 9.99362-01 KGS.

           PH =        1.631          IONIC STRENGTH = 2.05425-01          RES. E.N. =   2.666-11
```

```
                                           RUN 106
                                                              TEMPFRATURE    25.000  DEG. C
03 AUG 71    11:09:49.517
                                        INPUT MOLES

 SO2  =0.00000
 CO2  =0.00000
 SO3  =0.00000          N205 =1.00000-01    CAO  =0.00000       MGO  =0.00000
 NA2O =9.80000-02       HCL  =0.00000       H2O  =5.57207+01    N203 =1.67000-02


                                  AQUEOUS SOLUTION EQUILIBRIA

            COMPONENT          MOLALITY            ACTIVITY        ACTIVITY COEFFICIENT
                                                                         9.932-01
            H2O                                                          8.312-01
            H+                 2.811-02            2.336-02              7.437-01
            OH-                5.791-13            4.306-13              6.316-01
            NO3-               1.933-01            1.221-01              7.546-01
            NA+                1.894-01            1.429-01              1.037+00
            NAOH               1.596-14            1.657-14              1.037+00
            NANO3              6.703-03            6.949-03              1.037+00
            HNO3               1.074-04            1.113-04              6.316-01
            NO2-               2.421-02            1.529-02              1.037+00
            HNO2               4.761-01            4.936-01

                              MOLECULAR WATER = 9.99324-01 KGS.

      PH =        1.631         IONIC STRENGTH = 2.05432-01          RES. E.N. =  -1.034-11
```

```
                                           RUN 109
                                                              TEMPFRATURE    25.000  DEG. C
03 AUG 71    11:09:49.886
                                        INPUT MOLES

 SO2  =0.00000
 CO2  =0.00000
 SO3  =0.00000          N205 =1.00000-01    CAO  =0.00000       MGO  =0.00000
 NA2O =1.40000-02       HCL  =0.00000       H2O  =5.55382+01    N203 =1.81500-02


                                  AQUEOUS SOLUTION EQUILIBRIA

            COMPONENT          MOLALITY            ACTIVITY        ACTIVITY COEFFICIENT
                                                                         9.933-01
            H2O                                                          8.308-01
            H+                 1.763-01            1.465-01              7.445-01
            OH-                9.229-14            6.870-14              6.342-01
            NO3-               1.994-01            1.265-01              7.556-01
            NA+                2.716-02            2.052-02              1.036+00
            NAOH               3.663-16            3.794-16              1.036+00
            NANO3              9.972-04            1.033-03              1.036+00
            HNO3               6.975-04            7.225-04              6.342-01
            NO2-               4.027-03            2.554-03              1.036+00
            HNO2               4.987-01            5.166-01

                              MOLECULAR WATER = 9.94523-01 KGS.

      PH =         .834         IONIC STRENGTH = 2.01421-01          RES. E.N. =  -1.411-09
```

```
                                                     RUN 108
03 AUG 71     11:09:50.861                                                 TEMPERATURE    25.000  DEG. C
                                              INPUT MOLES

 SO2  =0.00000
 CO2  =0.00000
 SO3  =0.00000          N2O5 =1.00000-01     CAO  =0.00000       MGO  =0.00000
 NA2O =1.40000-02       HCL  =0.00000        H2O  =5.55364+01    N2O3 =1.63500-02


                                         AQUEOUS SOLUTION EQUILIBRIA

                 COMPONENT           MOLALITY            ACTIVITY        ACTIVITY COEFFICIENT
                 H2O                                                          9.933-01
                 H+                  1.763-01            1.465-01             8.308-01
                 OH-                 9.228-14            6.870-14             7.445-01
                 NO3-                1.994-01            1.265-01             6.342-01
                 NA+                 2.716-02            2.052-02             7.556-01
                 NAOH                3.663-16            3.794-16             1.036+00
                 NANO3               9.972-04            1.033-03             1.036+00
                 HNO3                6.975-04            7.225-04             1.036+00
                 NO2-                4.027-03            2.554-03             6.342-01
                 HNO2                4.987-01            5.166-01             1.036+00

                                         MOLECULAR WATER = 9.94490-01 KGS.

                   PH =        .834          IONIC STRENGTH = 2.01427-01            RES. E.N. =  -1.263-11
```

```
                                                     RUN 12
03 AUG 71     11:09:51.230                                                 TEMPERATURE    25.000  DEG. C
                                              INPUT MOLES

 SO2  =0.00000
 CO2  =0.00000
 SO3  =0.00000          N2O5 =3.17500-01     CAO  =0.00000       MGO  =0.00000
 NA2O =0.00000          HCL  =0.00000        H2O  =5.59128+01    N2O3 =8.92500-02


                                         AQUEOUS SOLUTION EQUILIBRIA

                 COMPONENT           MOLALITY            ACTIVITY        ACTIVITY COEFFICIENT
                 H2O                                                          9.793-01
                 H+                  6.322-01            5.914-01             9.354-01
                 OH-                 2.267-14            1.677-14             7.399-01
                 NO3-                6.308-01            2.940-01             4.662-01
                 HNO3                6.074-03            6.784-03             1.117+00
                 NO2-                1.466-03            6.835-04             4.662-01
                 HNO2                5.000-01            5.584-01             1.117+00

                                         MOLECULAR WATER = 9.97101-01 KGS.

                   PH =        .228          IONIC STRENGTH = 6.31507-01            RES. E.N. =  -4.155-12
```

```
                                                      RUN 13
03 AUG 71    11:09:51.864                                                   TEMPFRATURE    25.000  DEG. C
                                             INPUT MOLES

 SO2  =0.00000
 CO2  =0.00000
 SO3  =0.00000        N205 =3.17500-01    CAO  =0.00000       MGO  =0.00000
 NA2O =0.00000        HCL  =0.00000       H2O  =5.59083+01    N203 =8.48000-02


                                        AQUEOUS SOLUTION EQUILIBRIA

           COMPONENT          MOLALITY              ACTIVITY        ACTIVITY COEFFICIENT
           H2O                                                          9.793-01
           H+                6.323-01              5.915-01             9.354-01
           OH-               2.267-14              1.677-14             7.399-01
           NO3-              6.308-01              2.941-01             4.662-01
           HNO3              6.075-03              6.785-03             1.117+00
           NO2-              1.466-03              6.835-04             4.662-01
           HNO2              5.000-01              5.585-01             1.117+00

                                        MOLECULAR WATER = 9.97020-01 KGS.

           PH =        .228          IONIC STRENGTH = 6.31558-01           RES. E.N. =  -1.293-11
```

```
                                                      RUN 11
03 AUG 71    11:09:52.177                                                   TEMPERATURE    25.000  DEG. C
                                             INPUT MOLES

 SO2  =0.00000
 CO2  =0.00000
 SO3  =0.00000        N205 =3.17500-01    CAO  =0.00000       MGO  =0.00000
 NA2O =0.00000        HCL  =0.00000       H2O  =5.59065+01    N203 =6.30000-02


                                        AQUEOUS SOLUTION EQUILIBRIA

           COMPONENT          MOLALITY              ACTIVITY        ACTIVITY COEFFICIENT
           H2O                                                          9.793-01
           H+                6.323-01              5.915-01             9.354-01
           OH-               2.267-14              1.677-14             7.399-01
           NO3-              6.308-01              2.941-01             4.661-01
           HNO3              6.076-03              6.786-03             1.117+00
           NO2-              1.466-03              6.835-04             4.661-01
           HNO2              5.000-01              5.585-01             1.117+00

                                        MOLECULAR WATER = 9.96987-01 KGS.

           PH =        .228          IONIC STRENGTH = 6.31578-01           RES. E.N. =  -3.404-12
```

```
03 AUG 71    11:09:52.490                       RUN 14
                                           INPUT MOLES                    TEMPERATURE    25.000  DEG. C

 SO2  =0.00000
 CO2  =0.00000
 SO3  =0.00000        N2O5 =3.17500-01    CAO  =0.00000      MGO  =0.00000
 NA2O =0.00000        HCL  =0.00000       H2O  =5.59035+01   N2O3 =8.00000-02


                                  AQUEOUS SOLUTION EQUILIBRIA

             COMPONENT          MOLALITY            ACTIVITY       ACTIVITY COEFFICIENT
             H2O                                                        9.793-01
             H+                 6.323-01            5.915-01            9.354-01
             OH-                2.267-14            1.677-14            7.399-01
             NO3-               6.309-01            2.941-01            4.661-01
             HNO3               6.076-03            6.786-03            1.117+00
             NO2-               1.466-03            6.835-04            4.661-01
             HNO2               5.001-01            5.585-01            1.117+00

                                  MOLECULAR WATER = 9.96933-01 KGS.

             PH =       .228          IONIC STRENGTH = 6.31612-01          RES. E.N. =  -6.961-12
```

```
03 AUG 71    11:09:52.803                       RUN 92
                                           INPUT MOLES                    TEMPERATURE    25.000  DEG. C

 SO2  =0.00000
 CO2  =0.00000
 SO3  =0.00000        N2O5 =3.50000-01    CAO  =0.00000      MGO  =0.00000
 NA2O =2.00000-01     HCL  =0.00000       H2O  =5.62044+01   N2O3 =1.48400-01


                                  AQUEOUS SOLUTION EQUILIBRIA

             COMPONENT          MOLALITY            ACTIVITY       ACTIVITY COEFFICIENT
             H2O                                                        9.784-01
             H+                 2.985-01            2.828-01            9.473-01
             OH-                4.716-14            3.505-14            7.431-01
             NO3-               6.647-01            3.040-01            4.574-01
             NA+                3.693-01            2.650-01            7.176-01
             NAOH               2.225-15            2.500-15            1.124+00
             NANO3              2.855-02            3.208-02            1.124+00
             HNO3               2.985-03            3.354-03            1.124+00
             NO2-               3.108-03            1.422-03            4.574-01
             HNO2               4.942-01            5.553-01            1.124+00

                                  MOLECULAR WATER = 1.00537+00 KGS.

             PH =       .549          IONIC STRENGTH = 6.66283-01          RES. E.N. =   3.293-11
```

RUN 93

```
                                                                   TEMPERATURE    25.000  DEG. C
03 AUG 71     11:09:53.778                    INPUT MOLES

 SO2  =0.00000
 CO2  =0.00000
 SO3  =0.00000           N2O5 =3.50000-01    CAO  =0.00000        MGO  =0.00000
 NA2O =1.25000-01        HCL  =0.00000       H2O  =5.60931+01     N2O3 =1.12150-01

                                   AQUEOUS SOLUTION EQUILIBRIA

           COMPONENT          MOLALITY              ACTIVITY         ACTIVITY COEFFICIENT
           H2O                                                           9.780-01
           H+                 4.467-01              4.248-01             9.510-01
           OH-                3.134-14              2.332-14             7.442-01
           NO3-               6.760-01              3.074-01             4.547-01
           NA+                2.314-01              1.661-01             7.175-01
           NAOH               9.259-16              1.042-15             1.126+00
           NANO3              1.805-02              2.032-02             1.126+00
           HNO3               4.525-03              5.094-03             1.126+00
           NO2-               2.097-03              9.533-04             4.547-01
           HNO2               4.969-01              5.594-01             1.126+00

                                   MOLECULAR WATER = 1.00202+00 KGS.

            PH =        .372        IONIC STRENGTH = 6.77065-01          RES. E.N. =   1.534-09
```

RUN 94

```
                                                                   TEMPERATURE    25.000  DEG. C
03 AUG 71     11:09:54.599                    INPUT MOLES

 SO2  =0.00000
 CO2  =0.00000
 SO3  =0.00000           N2O5 =3.50000-01    CAO  =0.00000        MGO  =0.00000
 NA2O =1.25000-01        HCL  =0.00000       H2O  =5.60892+01     N2O3 =1.08250-01

                                   AQUEOUS SOLUTION EQUILIBRIA

           COMPONENT          MOLALITY              ACTIVITY         ACTIVITY COEFFICIENT
           H2O                                                           9.780-01
           H+                 4.467-01              4.248-01             9.510-01
           OH-                3.133-14              2.332-14             7.442-01
           NO3-               6.761-01              3.074-01             4.547-01
           NA+                2.315-01              1.661-01             7.175-01
           NAOH               9.259-16              1.042-15             1.126+00
           NANO3              1.805-02              2.033-02             1.126+00
           HNO3               4.525-03              5.095-03             1.126+00
           NO2-               2.097-03              9.533-04             4.547-01
           HNO2               4.969-01              5.594-01             1.126+00

                                   MOLECULAR WATER = 1.00195+00 KGS.

            PH =        .372        IONIC STRENGTH = 6.77110-01          RES. E.N. =  -1.392-11
```

RUN 78

```
03 AUG 71    11:09:55.472                                          TEMPFRATURE    25.000  DEG. C
                                     INPUT MOLES

 SO2  =0.00000
 CO2  =0.00000
 SO3  =0.00000       N205 =3.50000-01    CAO  =0.00000       MGO  =0.00000
 NA2O =7.30000-02    HCL  =0.00000       H2O  =5.60051+01    N2O3 =7.61000-02

                              AQUEOUS SOLUTION EQUILIBRIA

          COMPONENT          MOLALITY            ACTIVITY       ACTIVITY COEFFICIENT
          H2O                                                        9.776-01
          H+                 5.504-01            5.249-01            9.538-01
          OH-                2.532-14            1.887-14            7.450-01
          NO3-               6.841-01            3.098-01            4.528-01
          NA+                1.354-01            9.718-02            7.175-01
          NAOH               4.377-16            4.934-16            1.127+00
          NANO3              1.063-02            1.198-02            1.127+00
          HNO3               5.627-03            6.343-03            1.127+00
          NO2-               1.712-03            7.751-04            4.528-01
          HNO2               4.985-01            5.620-01            1.127+00

                          MOLECULAR WATER = 9.99493-01 KGS.

            PH =        .280          IONIC STRENGTH = 6.84956-01          RES. E.N. =  -4.438-12
```

RUN 80

```
03 AUG 71    11:09:56.203                                          TEMPERATURE    25.000  DEG. C
                                     INPUT MOLES

 SO2  =0.00000
 CO2  =0.00000
 SO3  =0.00000       N205 =3.50000-01    CAO  =0.00000       MGO  =0.00000
 NA2O =7.30000-02    HCL  =0.00000       H2O  =5.60035+01    N2O3 =7.45500-02

                              AQUEOUS SOLUTION EQUILIBRIA

          COMPONENT          MOLALITY            ACTIVITY       ACTIVITY COEFFICIENT
          H2O                                                        9.776-01
          H+                 5.504-01            5.249-01            9.538-01
          OH-                2.532-14            1.886-14            7.450-01
          NO3-               6.841-01            3.098-01            4.528-01
          NA+                1.354-01            9.718-02            7.175-01
          NAOH               4.377-16            4.934-16            1.127+00
          NANO3              1.063-02            1.198-02            1.127+00
          HNO3               5.627-03            6.344-03            1.127+00
          NO2-               1.712-03            7.751-04            4.528-01
          HNO2               4.986-01            5.620-01            1.127+00

                          MOLECULAR WATER = 9.99465-01 KGS.

            PH =        .280          IONIC STRENGTH = 6.84974-01          RES. E.N. =  -3.697-12
```

```
                                        RUN 81

03 AUG 71    11:09:56.572                                       TEMPERATURE    25.000  DEG. C
                                   INPUT MOLES

[illegible]  =0.00000
[illegible]  =0.00000
[illegible]  =0.00000        N205 =3.50000-01    CAO  =0.00000       MGO  =0.00000
NA2[illegible] =7.30000-02   HCL  =0.0000U       H2O  =5.60034+01    N2O3 =7.44000-02

                               AQUEOUS SOLUTION EQUILIBRIA

          COMPONENT          MOLALITY            ACTIVITY       ACTIVITY COEFFICIENT
          H2O                                                          9.776-01
          H+                5.504-01            5.249-01              9.536-01
          OH-               2.532-14            1.686-14              7.450-01
          NO3-              6.841-01            3.098-01              4.528-01
          NA+               1.354-01            9.718-02              7.175-01
          NAOH              4.377-16            4.934-16              1.127+00
          NANO3             1.063-02            1.198-02              1.127+00
          HNO3              5.627-03            6.344-03              1.127+00
          NO2-              1.712-03            7.751-04              4.528-01
          HNO2              4.986-01            5.620-01              1.127+00

                         MOLECULAR WATER = 9.99463-01 KGS.

     PH =        .280          IONIC STRENGTH = 6.84976-01           RES. E.N. =  -2.878-13
```

```
                                        RUN 68

03 AUG 71    11:09:56.847                                       TEMPERATURE    25.000  DEG. C
                                   INPUT MOLES

SO2  =0.00000
CO2  =0.00000
SO3  =0.00000        N205 =3.50000-01    CAO  =0.00000       MGO  =0.00000
NA2O =2.30000-01     HCL  =0.00000       H2O  =5.61430+01    N2O3 =5.70500-02

                               AQUEOUS SOLUTION EQUILIBRIA

          COMPONENT          MOLALITY            ACTIVITY       ACTIVITY COEFFICIENT
          H2O                                                          9.786-01
          H+                2.403-01            2.274-01              9.463-01
          OH-               5.868-14            4.359-14              7.428-01
          NO3-              6.615-01            3.030-01              4.581-01
          NA+               4.250-01            3.050-01              7.177-01
          NAOH              3.187-15            3.579-15              1.123+00
          NANO3             3.276-02            3.680-02              1.123+00
          HNO3              2.394-03            2.688-03              1.123+00
          NO2-              3.854-03            1.765-03              4.581-01
          HNO2              4.936-01            5.545-01              1.123+00

                         MOLECULAR WATER = 1.00481+00 KGS.

     PH =        .643          IONIC STRENGTH = 6.63423-01           RES. E.N. =  -1.033-11
```

RUN 66

```
03 AUG 71    11:09:57.822                                    TEMPERATURE    25.000  DEG. C
                                     INPUT MOLES

SO2  =0.00000
CO2  =0.00000
SO3  =0.00000       N2O5 =3.50000-01    CAO  =0.00000      MGO  =0.00000
NA2O =2.30000-01    HCL  =0.00000       H2O  =5.61428+01   N2O3 =5.68000-02

                              AQUEOUS SOLUTION EQUILIBRIA

          COMPONENT         MOLALITY           ACTIVITY       ACTIVITY COEFFICIENT
          H2O                                                     9.786-01
          H+                2.403-01           2.274-01           9.463-01
          OH-               5.868-14           4.359-14           7.428-01
          NO3-              6.615-01           3.030-01           4.581-01
          NA+               4.250-01           3.050-01           7.177-01
          NAOH              3.187-15           3.579-15           1.123+00
          NANO3             3.276-02           3.680-02           1.123+00
          HNO3              2.394-03           2.688-03           1.123+00
          NO2-              3.854-03           1.765-03           4.581-01
          HNO2              4.938-01           5.545-01           1.123+00

                          MOLECULAR WATER = 1.00480+00 KGS.

           PH =       .643          IONIC STRENGTH = 6.63425-01          RES. E.N. =  -1.022-12
```

RUN 69

```
03 AUG 71    11:09:58.099                                    TEMPERATURE    25.000  DEG. C
                                     INPUT MOLES

SO2  =0.00000
CO2  =0.00000
SO3  =0.00000       N2O5 =3.50000-01    CAO  =0.00000      MGO  =0.00000
NA2O =2.30000-01    HCL  =0.00000       H2O  =5.61389+01   N2O3 =5.29500-02

                              AQUEOUS SOLUTION EQUILIBRIA

          COMPONENT         MOLALITY           ACTIVITY       ACTIVITY COEFFICIENT
          H2O                                                     9.786-01
          H+                2.403-01           2.274-01           9.463-01
          OH-               5.867-14           4.359-14           7.428-01
          NO3-              6.615-01           3.030-01           4.581-01
          NA+               4.251-01           3.051-01           7.177-01
          NAOH              3.166-15           3.579-15           1.123+00
          NANO3             3.277-02           3.680-02           1.123+00
          HNO3              2.394-03           2.689-03           1.123+00
          NO2-              3.854-03           1.765-03           4.581-01
          HNO2              4.938-01           5.546-01           1.123+00

                          MOLECULAR WATER = 1.00473+00 KGS.

           PH =       .643          IONIC STRENGTH = 6.63469-01          RES. E.N. =  -2.509-11
```

RUNS 87 and 88

```
                                                                   TEMPERATURE    25.000  DEG. C
03 AUG 71     11:09:58.467                        INPUT MOLES

 SO2  =0.00000
 CO2  =0.00000
 SO3  =0.00000         N205 =3.50000-01     CAO  =0.00000        MGO  =0.00000
 NA2O =3.07500-01      HCL  =0.00000        H2O  =5.62034+01     N2O3 =3.99500-02

                                         AQUEOUS SOLUTION EQUILIBRIA

                 COMPONENT          MOLALITY            ACTIVITY       ACTIVITY COEFFICIENT
                 H2O                                                        9.789-01
                 H+                 9.323-02            8.797-02            9.436-01
                 OH-                1.519-13            1.127-13            7.421-01
                 NO3-               6.508-01            2.994-01            4.600-01
                 NA+                5.673-01            4.072-01            7.178-01
                 NAOH               1.101-14            1.235-14            1.122+00
                 NANO3              4.327-02            4.853-02            1.122+00
                 HNO3               9.160-04            1.027-03            1.122+00
                 NO2-               9.763-03            4.491-03            4.600-01
                 HNO2               4.866-01            5.458-01            1.122+00

                                     MOLECULAR WATER = 1.00729+00 KGS.

                  PH =       1.056          IONIC STRENGTH = 6.55635-01          RES. E.N. =  -1.048-11
```

RUNS 97 and 98

```
                                                                   TEMPFRATURE    25.000  DEG. C
03 AUG 71     11:09:59.352                        INPUT MOLES

 SO2  =0.00000
 CO2  =0.00000
 SO3  =0.00000         N205 =3.50000-01     CAO  =0.00000        MGO  =0.00000
 NA2O =3.40000-01      HCL  =0.00000        H2O  =5.62300+01     N2O3 =3.40000-02

                                         AQUEOUS SOLUTION EQUILIBRIA

                 COMPONENT          MOLALITY            ACTIVITY       ACTIVITY COEFFICIENT
                 H2O                                                        9.789-01
                 H+                 4.105-02            3.876-02            9.441-01
                 OH-                3.447-13            2.558-13            7.422-01
                 NO3-               6.464-01            2.971-01            4.596-01
                 NA+                6.269-01            4.500-01            7.177-01
                 NAOH               2.762-14            3.098-14            1.122+00
                 NANO3              4.744-02            5.322-02            1.122+00
                 HNO3               4.004-04            4.492-04            1.122+00
                 NO2-               2.162-02            9.937-03            4.596-01
                 HNO2               4.742-01            5.320-01            1.122+00

                                     MOLECULAR WATER = 1.00836+00 KGS.

                  PH =       1.412          IONIC STRENGTH = 6.57173-01          RES. E.N. =   1.374-10
```

```
                                        RUN 99
 03 AUG 71    11:10:00.173                                       TEMPERATURE    25.000  DEG. C
                                   INPUT MOLES

  SO2  =0.00000
  CO2  =0.00000
  SO3  =0.00000       N2O5 =3.50000-01    CAO  =0.00000      MGO  =0.00000
  NA2O =2.78500-01    HCL  =0.00000       H2O  =5.61514+01   N2O3 =1.69500-02

                              AQUEOUS SOLUTION EQUILIBRIA

          COMPONENT         MOLALITY            ACTIVITY       ACTIVITY COEFFICIENT
          H2O                                                       9.788-01
          H+                1.470-01            1.388-01            9.445-01
          OH-               9.622-14            7.143-14            7.423-01
          NO3-              6.551-01            3.009-01            4.594-01
          NA+               5.144-01            3.692-01            7.177-01
          NAOH              6.325-15            7.097-15            1.122+00
          NANO3             3.941-02            4.423-02            1.122+00
          HNO3              1.452-03            1.630-03            1.122+00
          NO2-              6.253-03            2.872-03            4.594-01
          HNO2              4.908-01            5.508-01            1.122+00

                            MOLECULAR WATER = 1.00583+00 KGS.

            PH =        .858          IONIC STRENGTH = 6.58202-01           RES. E.N. =  -8.052-13
```

```
                                        RUN 124
 03 AUG 71    11:10:01.879                                       TEMPERATURE    25.000  DEG. C
                                   INPUT MOLES

  SO2  =0.00000
  CO2  =0.00000
  SO3  =0.00000       N2O5 =6.25000-01    CAO  =0.00000      MGO  =0.00000
  NA2O =1 50000-01    HCL  =0.00000       H2O  =5.64147+01   N2O3 =1.33700-01

                              AQUEOUS SOLUTION EQUILIBRIA

          COMPONENT         MOLALITY            ACTIVITY       ACTIVITY COEFFICIENT
          H2O                                                       9.604-01
          H+                9.332-01            1.094+00            1.173+00
          OH-               1.060-14            8.690-15            8.230-01
          NO3-              1.204+00            4.280-01            3.556-01
          NA+               2.717-01            1.976-01            7.270-01
          NAOH              3.829-16            4.727-16            1.235+00
          NANO3             2.727-02            3.367-02            1.235+00
          HNO3              1.480-02            1.827-02            1.235+00
          NO2-              1.142-03            4.061-04            3.556-01
          HNO2              4.972-01            6.139-01            1.235+00

                            MOLECULAR WATER = 1.00331+00 KGS.

            PH =       -.039          IONIC STRENGTH = 1.20439+00           RES. E.N. =   4.255-11
```

```
03 AUG 71     11:10:03.003                RUNS 120 and 121          TEMPERATURE    25.000  DEG. C
                                        INPUT MOLES

 SO2  =0.00000
 CO2  =0.00000
 SO3  =0.00000          N2O5 =6[illegible]00-01    CAO  =0.00000        MGO  =0.00000
 NA2O =1.00000-01       HCL  =[illegible]000       H2O  =5.63370+01     N2O3 =1.06000-01


                                 AQUEOUS SOLUTION EQUILIBRIA

            COMPONENT          MOLALITY              ACTIVITY        ACTIVITY COEFFICIENT
            H2O                                                           9.599-01
            H+                 1.033+00              1.217+00            1.178+00
            OH-                9.685-15              7.989-15            8.249-01
            NO3-               1.214+00              4.298-01            3.541-01
            NA+                1.815-01              1.320-01            7.274-01
            NAOH               2.296-16              2.839-16            1.237+00
            NANO3              1.827-02              2.260-02            1.237+00
            HNO3               1.650-02              2.041-02            1.237+00
            NO2-               1.036-03              3.667-04            3.541-01
            HNO2               4.985-01              6.165-01            1.237+00

                           MOLECULAR WATER = 1.00100+00 KGS.

       PH =        -.085          IONIC STRENGTH = 1.21450+00            RES. E.N. =   4.424-12
```

```
                                          RUNS 129 and 130
03 AUG 71     11:10:03.824                                            TEMPERATURE    25.000  DEG. C
                                        INPUT MOLES

 SO2  =0.00000
 CO2  =0.00000
 SO3  =0.00000          N2O5 =4.47000-01    CAO  =0.00000        MGO  =0.00000
 NA2O =1.00000-01       HCL  =0.00000       H2O  =5.61384+01     N2O3 =8.54500-02


                                 AQUEOUS SOLUTION EQUILIBRIA

            COMPONENT          MOLALITY              ACTIVITY        ACTIVITY COEFFICIENT
            H2O                                                           9.716-01
            H+                 6.866-01              7.026-01            1.023+00
            OH-                1.825-14              1.401-14            7.676-01
            NO3-               8.688-01              3.585-01            4.126-01
            NA+                1.837-01              1.320-01            7.183-01
            NAOH               4.272-16              4.974-16            1.164+00
            NANO3              1.617-02              1.883-02            1.164+00
            HNO3               8.439-03              9.826-03            1.164+00
            NO2-               1.449-03              5.977-04            4.126-01
            HNO2               4.982-01              5.801-01            1.164+00

                           MOLECULAR WATER = 1.00063+00 KGS.

       PH =        .153           IONIC STRENGTH = 8.69549-01            RES. E.N. =  -1.125-12
```

RUNS 122 and 123

```
03 AUG 71    11:10:04.646                                           TEMPERATURE    25.000  DEG. C
                                           INPUT MOLES

 SO2  =0.00000
 CO2  =0.00000
 SO3  =0.00000       N2O5 =6.25000-01     CAO  =0.00000       MGO  =0.00000
 NA2O =5.68000-01    HCL  =0.00000        H2O  =5.67476+01    N2O3 =4.86000-02


                                   AQUEOUS SOLUTION EQUILIBRIA

             COMPONENT          MOLALITY              ACTIVITY       ACTIVITY COEFFICIENT
             H2O                                                          9.643-01
             H+                 1.189-01              1.353-01            1.138+00
             OH-                6.913-14              7.217-14            8.097-01
             NO3-               1.126+00              4.134-01            3.665-01
             NA+                1.018+00              7.374-01            7.246-01
             NAOH               1.175-14              1.432-14            1.219+00
             NANO3              9.955-02              1.214-01            1.219+00
             HNO3               1.790-03              2.183-03            1.219+00
             NO2-               8.596-03              3.151-03            3.665-01
             HNO2               4.831-01              5.690-01            1.219+00

                                   MOLECULAR WATER = 1.01683+00 KGS.

               PH =       .869          IONIC STRENGTH = 1.13227+00            RES. E.N. =  -5.555-14
```

RUNS 61 and 62

```
03 AUG 71    11:10:05.826                                           TEMPERATURE    25.000  DEG. C
                                           INPUT MOLES

 SO2  =0.00000
 CO2  =0.00000
 SO3  =0.00000       N2O5 =5.82500-01     CAO  =0.00000       MGO  =0.00000
 NA2O =2.00000-02    HCL  =0.00000        H2O  =5.61284+01    N2O3 =1.99500-02


                                   AQUEOUS SOLUTION EQUILIBRIA

             COMPONENT          MOLALITY              ACTIVITY       ACTIVITY COEFFICIENT
             H2O                                                          9.619-01
             H+                 1.113+00              1.275+00            1.146+00
             OH-                9.401-15              7.641-15            8.127-01
             NO3-               1.148+00              4.180-01            3.639-01
             NA+                3.653-02              2.649-02            7.251-01
             NAOH               4.456-17              5.448-17            1.223+00
             NANO3              3.605-03              4.408-03            1.223+00
             HNO3               1.701-02              2.079-02            1.223+00
             NO2-               9.551-04              3.476-04            3.639-01
             HNO2               5.008-01              6.123-01            1.223+00

                                   MOLECULAR WATER = 9.96572-01 KGS.

               PH =      -.106          IONIC STRENGTH = 1.14888+00            RES. E.N. =  -7.929-12
```

The vapor phase data were reported in units of atmospheres of N^{+3}. The equilibrium constant for reaction (21) was calculated from standard state thermodynamic properties at 25°C and is given in equation (29).

$$K_{25°C} = \frac{P_{HNO_2}^2}{P_{N_2O_3}P_{H_2O}} = .6466 \qquad (29)$$

The vapor pressure of water at 25°C is 23.756 mm or .0313 atm. Substituting in (29) gives (30)

$$P_{H_2O}K_{25°C} = \frac{P_{HNO_2}^2}{P_{N_2O_3}} = .0202 \qquad (30)$$

The total measured pressure is the sum of pressures of HNO_2 and N_2O_3 as shown in (31)

$$P_{meas} = P_{HNO_2} + 2P_{N_2O_3} \qquad (31)$$

Substituting (30) in (31) gives (32).

$$P_{meas} = P_{HNO_2} + \frac{2P_{HNO_2}^2}{.0202} \qquad (32)$$

Equation (32) can be solved using the quadratic formula and the measured values of P as in (33).

$$P_{HNO_2} = \frac{-.0202 + \quad .000408 + .1616\ P_{meas}}{4} \qquad (33)$$

The results are given in Table VII along with the corrected value of K which was calculated using the activities in Table VI.

TABLE VII

Calculated Values of P_{HNO_2} and K_{corr} from the

Date of Abel and Neusser (AB-006)

Run No. (from AB-006)	P_{meas} (atm)	P_{HNO_2} (atm)	$K_{corr} = \frac{a_{H^+}a_{NO_2^-}}{P_{HNO_2}}$
112	.00462	.00344	.107
113	.00439	.00331	.111
105	.00316	.00253	.147
103	.00319	.00255	.146
102	.00284	.00231	.161
107	.00175	.00152	.235
106	.00189	.00163	.219
109	.00154	.00135	.276
108	.00141	.00125	.298
12	.00528	.00382	.106
13	.00590	.00417	.097
11	.00608	.00427	.095
14	.00552	.00396	.102
92	.01113	.00669	.060
93	.00721	.00486	.083
94	.00767	.00509	.079
78	.00495	.00364	.112
80	.00450	.00337	.121
81	.00506	.00370	.110
68	.00360	.00281	.143
69	.00366	.00285	.141
66	.00370	.00288	.139
87	.00268	.00220	.180

TABLE VII (Continued)

Run No. (from AB-006)	P_{meas} (atm)	P_{HNO_3} (atm)	$K_{corr} = \frac{a_{H^+}a_{NO_3^-}}{P_{HNO_3}}$
88	.00272	.00223	.177
97	.00221	.00187	.207
98	.00205	.00174	.221
99	.00118	.00107	.374
124	.00921	.00584	.076
120	.00818	.00535	.083
121	.00815	.00533	.084
129	.00700	.00476	.088
130	.00702	.00477	.088
122	.00408	.00312	.137
123	.00414	.00315	.135
61	.00116	.00105	.422
62	.00120	.00108	.409

avg. $K_{corr} = 0.160 \pm .09$

The slope of a graph of ln P_{HNO_3} vs. ln $a_{H^+}a_{NO_3^-}$ gave essentially the same value for K as the average value K = 0.160.

The vapor-liquid equilibrium constant, $K = a_{HNO_3(\ell)}/a_{HNO_3(g)}$ can be calculated from K_{corr} as shown in equations (34) through (36).

$$K_{corr} = \frac{a_{H^+}a_{NO_3^-}}{P_{HNO_3}} \qquad (34)$$

$$K_{diss} = \frac{a_{H^+}a_{NO_3^-}}{a_{HNO_3(\ell)}} \qquad (35)$$

$$K = \frac{K_{corr}}{K_{diss}} = \frac{a_{HNO_3(\ell)}}{P_{HNO_3(g)}} \cong \frac{a_{HNO_3(\ell)}}{a_{HNO_3(g)}} \qquad (36)$$

Using the value of $K_{diss,25°C} = 7.24 \times 10^{-4}$ given in Section 3.2, Table IV, K is calculated to be 2.155×10^{2}.

3.3 Vapor-Liquid Equilibrium Constant for Nitric Acid

Vapor pressure measurements for HNO_3 have been conducted by numerous workers. However, the nitric acid solutions for which values of P_{HNO_3} are high enough to be measurable are in the concentration range 24 to 70 weight % (5. to 36. molal). This means the back pressure of HNO_3 over dilute solutions is essentially zero.

The data of Prosek (PR-009), McKeown and Belles (MC-035), Burdick and Freed (BU-014), Flatt and Benguerel (FL-013), Sproesser and Taylor (SP-006) and Davis and deBruin (DA-012) were considered. Only the data of Davis and deBruin were applicable, since the other values were measured over solutions of high ionic strength (I>5). Davis and deBruin measured the molality of NO_3^- and P_{HNO_3}. Using the equilibrium model, activities of H^+, NO_3^- and $HNO_{3(\ell)}$ were calculated from their molality data. The vapor-liquid equilibrium constant was then calculated using the six data points taken at ionic strengths of 6.7 and below. The results are given in Tables VIII and IX.

TABLE VIII

Results Obtained Using Radian's Aqueous Equilibrium Program to Calculate Activity of Nitric Acid

```
29 JUN 71    11:11:55.436                                          TEMPERATURE    25.000  DEG. C
                                         INPUT MOLES

 SO2  =0.00000
 CO2  =0.00000
 SO3  =0.00000      N2O5 =1.14294+00    CAO  =0,00000      MGO  =0.00000
 NA2O =0.00000      HCL  =0.00000       H2O  =5.66487+01   N2O3 =0.00000

                                 AQUEOUS SOLUTION EQUILIBRIA

            COMPONENT        MOLALITY            ACTIVITY        ACTIVITY COEFFICIENT
            H2O                                                       9.231-01
            H+               2.226+00            4.071+00             1.829+00
            OH-              2.12A-15            2.297-15             1.079+00
            NO3-             2.226+00            5.430-01             2.439-01
            HNO3             5.842-02            A.626-02             1.476+00

                                 MULECULAR WATER = 1.00000+00 KGS.

        PH =       -.610          IONIC STRENGTH = 2.22696+00           RES. E.N. =   8.829-11
```

```
29 JUN 71    11:11:56.109                                          TEMPERATURE    25.000  DEG. C
                                         INPUT MOLES

 SO2  =0.00000
 CO2  =0.00000
 SO3  =0.00000      N2O5 =1.62616+00    CAO  =0,00000      MGO  =0.00000
 NA2O =0.00000      HCL  =0.00000       H2O  =5.71324+01   N2O3 =0.00000

                                 AQUEOUS SOLUTION EQUILIBRIA

            COMPONENT        MOLALITY            ACTIVITY        ACTIVITY COEFFICIENT
            H2O                                                       8.860-01
            H+               3.141+00            8.672+00             2.761+00
            OH-              7.305-16            1.037-15             1.420+00
            NO3-             3.141+00            5.720-01             1.821-01
            HNO3             1.117-01            1.935-01             1.733+00

                                 MOLECULAR WATER = 1.00000+00 KGS.

        PH =       -.938          IONIC STRENGTH = 3.14064+00           RES. E.N. =  -2.696-11
```

```
29 JUN 71     11:11:56.657                                   TEMPERATURE    25.000  DEG. C
                                  INPUT MOLES

 SO2  =0.00000
 CO2  =0.00000
 SO3  =0.00000        N2O5 =1.64173+00    CAO  =0.00000      MGO  =0.00000
 NA2O =0.00000        HCL  =0.00000       H2O  =5.71480+01   N2O3 =0.00000


                           AQUEOUS SOLUTION EQUILIBRIA

            COMPONENT          MOLALITY            ACTIVITY       ACTIVITY COEFFICIENT
            H2O                                                        8.868-01
            H+                 3.170+00            8.869+00            2.798+00
            OH-                7.069-18            1.013-15            1.433+00
            NO3-               3.170+00            5.721-01            1.805-01
            HNO3               1.137-01            1.980-01            1.741+00

                           MOLECULAR WATER = 1.00000+00 KGS.

        PH =       -.948          IONIC STRENGTH = 3.16979+00           RES. E.N. =  -2.277-10
```

```
29 JUN 71     11:11:57.090                                   TEMPERATURE    25.000  DEG. C
                                  INPUT MOLES

 SO2  =0.00000
 CO2  =0.00000
 SO3  =0.00000        N2O5 =1.79207+00    CAO  =0.00000      MGO  =0.00000
 NA2O =0.00000        HCL  =0.00000       H2O  =5.72983+01   N2O3 =0.00000


                           AQUEOUS SOLUTION EQUILIBRIA

            COMPONENT          MOLALITY            ACTIVITY       ACTIVITY COEFFICIENT
            H2O                                                        8.757-01
            H+                 3.450+00            1.097+01            3.180+00
            OH-                5.170-16            8.085-16            1.564+00
            NO3-               3.450+00            5.721-01            1.658-01
            HNO3               1.339-01            2.448-01            1.829+00

                           MOLECULAR WATER = 1.00000+00 KGS.

        PH =      -1.040          IONIC STRENGTH = 3.45028+00           RES. E.N. =  -5.811-12
```

```
29 JUN 71    11:11:57.567                                              TEMPERATURE    25.000  DEG. C
                                      INPUT MOLES

 SO2   =0.00000
 CO2   =0.00000
 SO3   =0.00000        N2O5 =2.55413+00    CAO  =0.00000       MGO  =0.00000
 NA2O  =0.00000        HCL  =0.00000       H2O  =5,80609+01    N2O3 =0.00000

                              AQUEOUS SOLUTION EQUILIBRIA

           COMPONENT          MOLALITY             ACTIVITY        ACTIVITY COEFFICIENT
           H2O                                                            8.180-01
           H+                 4.896+00             2.926+01               6.037+00
           OH-                1.157-16             2.832-16               2.448+00
           NO3-               4.896+00             5.369-01               1.108-01
           HNO3               2.629-01             6.128-01               2.335+00

                              MOLECULAR WATER = 1.00000+00 KGS.

           PH =     -1.466          IONIC STRENGTH = 4.89582+00            RES. E.N. =  -8.074-12
```

```
29 JUN 71    11:11:58.043                                              TEMPERATURE    25.000  DEG. C
                                      INPUT MOLES

 SO2   =0.00000
 CO2   =0.00000
 SO3   =0.00000        N2O5 =3.58856+00    CAO  =0.00000       MGO  =0.00000
 NA2O  =0.00000        HCL  =0.00000       H2O  =5.90948+01    N2O3 =0.00000

                              AQUEOUS SOLUTION EQUILIBRIA

           COMPONENT          MOLALITY             ACTIVITY        ACTIVITY COEFFICIENT
           H2O                                                            7.389-01
           H+                 6.666+00             9.357+01               1.404+01
           OH-                1.787-17             7.999-17               4.475+00
           NO3-               6.666+00             4.496-01               6.744-02
           HNO3                .111-01             1.641+00               3.211+00

                              MOLECULAR WATER = 1.00000+00 KGS.

           PH =     -1.971          IONIC STRENGTH = 6.66605+00            RES. E.N. =   1.065-10
```

TABLE IX

Nitric Acid Vapor-Liquid Equilibrium
Constant Calculated from the Data of
Davis and deBruin (DA-012)

Calculated a_{H^+} (See Table VIII)	Calculated $a_{NO_3^-}$ (See Table VIII)	Measured P_{HNO_3} (atm x 10^7)	$K_{calc} = \frac{a_{H^+}a_{NO_3^-}}{P_{HNO_3}} \times 10^{-7}$
4.071	0.543	10.4	0.221
8.672	0.5720	29.0	0.171
8.869	0.5721	31.0	0.164
10.97	0.5721	51.0	0.123
29.26	0.5369	108.0	0.145
93.57	0.4496	386.0	0.109
		avg K_{calc} =	.156 x 10^7

A plot of ln $a_{H^+}a_{NO_3^-}$ vs. ln P_{HNO_3} had a slope of .151 x 10^7, while the average value of K_{calc} was .156 x 10^7.

The vapor liquid equilibrium constant for reaction (1a), $K = a_{HNO_3(\ell)}/a_{HNO_3(g)}$, can be calculated from the dissociation constant, K_{diss}, and the constant in Table IX as shown below.

$$K_{diss} = \frac{a_{H^+}a_{NO_3^-}}{a_{HNO_3(\ell)}} = 26.9 \qquad (38)$$

$$K_{calc} = \frac{a_{H^+}a_{NO_3^-}}{P_{HNO_3}} = .156 \times 10^7 \qquad (39)$$

$$K \cong \frac{a_{HNO_3(\ell)}}{P_{HNO_3(g)}} = \frac{K_{calc}}{K_{diss}} = 5.8 \times 10^4 \qquad (40)$$

3.4 Vapor-Liquid Equilibrium Constant for Nitric Oxide

The data of Winkler (WI-029) for the Bunsen absorption coefficient of NO in water were used to calculate the equilibrium constant for reaction (41).

$$NO_{(g)} \rightleftarrows NO_{(\ell)} \qquad (41)$$

The equilibrium constant is defined in equation (42) where the activity of $NO_{(\ell)}$ is in units of moles NO/kg H_2O, assuming $\gamma_{NO(\ell)} = 1$, and the activity of $NO_{(g)}$ is in units of atmospheres of nitric oxide.

$$K = \frac{a_{NO(\ell)}}{a_{NO(g)}} \qquad (42)$$

Winkler's data were reported in units of cc dissolved NO per cc water. He also reported the total measured pressure of nitric oxide over the solution in mm Hg. The number of moles of dissolved NO was calculated by multiplying Winkler's values of cc NO by $\left(\frac{10^{-3}\,\ell}{cc}\right)\left(\frac{mole}{22.4\,\ell}\right)$. The results of all the calculations are given in Table X. The data for each temperature are an average of three measurements.

TABLE X

Results of Calculation of Vapor-Liquid
Equilibrium Constant for Nitric Oxide from
the Data of Winkler (WI-029)

T°C	$CC_{NO}\left(\frac{10^{-3}\text{ moles}}{22.4\text{ cc}}\right)$ = moles NO	$CC_{H_2O}\left(\frac{10^{-3}\text{ kg}}{\text{cc}}\right)$ = kgH_2O	$\frac{\text{moles NO}}{\text{kg }H_2O} \cong a_{NO(\ell)}$	$P_{NO}\left(\frac{\text{atm}}{760\text{mm}}\right) \cong a_{NO(g)}$	$\frac{a_{NO(\ell)}}{P_{NO(g)}}$ =K
0.07	.00371	1.90505	.001947	.592	.00329
10.02	.00310	1.90532	.001626	.639	.00255
20.02	.00273	1.90813	.001495	.681	.00210
30.01	.00246	1.91292	.001289	.720	.00179
39.96	.00228	1.91946	.001188	.758	.00157
50.04	.00216	1.92762	.001124	.799	.00141
59.94	.00214	1.93700	.00110[illegible]	.838	.00132
70.05	.00215	1.94784	.001102	.879	.00125
79.85	.00217	1.95963	.001107	.919	.00120

4.0 SUMMARY

This Technical Note has described the selection of activity coefficients and equilibrium constants for use in an aqueous equilibrium model. The activity coefficients are correlated as a function of ionic strength. Correlation parameters for each ion or uncharged species were chosen on the basis of published graphs of activity coefficients as a function of ionic strength.

Equilibrium constants were selected from numerous different published references. In some cases the data were recalculated to obtain constants in a consistent form. The selected constants are listed in Table XI.

TABLE XI

Selected Values for Equilibrium Constants

Reaction	Form of Constant	Selected Values	Reference
$HNO_{3(\ell)} \rightleftarrows H^+ + NO_3^-$	$K = \frac{a_{H^+}a_{NO_3^-}}{a_{HNO_{3(\ell)}}}$	$K_{25°C} = 26.9$ $\log K = 6.557 - \frac{320.88}{T} - .01359T$	AE-001
$HNO_{3(g)} \rightleftarrows HNO_{3(\ell)}$	$K = \frac{a_{HNO_3(\ell)}}{P_{HNO_3(g)}}$	$K_{25°C} = 5.80 \times 10^4\ atm^{-1}$	DA-012
$HNO_{2(\ell)} \rightleftarrows H^+ + NO_2^-$	$K = \frac{a_{H^+}a_{NO_2^-}}{a_{HNO_{2(\ell)}}}$	$K_{25°C} = 7.24 \times 10^{-4}$ $\log K = 34.558 - \frac{5.8554 \times 10^3}{T} - 60.571 \times 10^{-3}T$	LU-005 TU-007
$HNO_{2(g)} \rightleftarrows HNO_{2(\ell)}$	$K = \frac{a_{HNO_2(\ell)}}{P_{HNO_2(g)}}$	$K_{25°C} = 2.155 \times 10^2\ atm^{-1}$	AB-006
$NO_{(g)} \rightleftarrows NO_{(\ell)}$	$K = \frac{a_{NO(\ell)}}{P_{NO(g)}}$	$K_{20°C} = 2.10 \times 10^{-3}\ atm^{-1}$	WI-029

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TECHNICAL NOTE 200-007-12

VAPOR FILM MASS TRANSFER COEFFICIENTS FOR HNO_2 AND HNO_3 IN A PACKED TOWER

1 November 1971

Prepared by:

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CHEMICAL RESEARCH • SYSTEMS ANALYSIS • COMPUTER SCIENCE • CHEMICAL ENGINEERING

1.0 INTRODUCTION

The sorption of nitrogen oxides in aqueous alkaline sorbents is the basis of a potential NO_x removal process. EPA has performed bench scale tests of the sorption of nitrogen oxides in their Cincinnati laboratories. In this technical note some of the experimental data are analyzed to extract mass transfer coefficients.

In support of the EPA program, Radian has made some theoretical calculations that indicate that HNO_2 and HNO_3 are the significant molecular species involved in the mass transfer step. The analysis presented is based on the assumption that mass transfer is vapor film limited. Not enough experimental data were taken to prove or disprove this assumption. The conclusions must therefore be treated as tentative.

2.0 THEORY

The general mass transfer theories apply to this problem. The major difference between standard computational schemes and what is presented here is that the species involved in the mass transfer process, i.e., HNO_2 and HNO_3 are not conserved species. For example, when HNO_2 is removed from the gas phase, more HNO_2 is formed as a result of the vapor phase reaction among the various nitrogen oxides and water.

A material balance may be made across a differential height of packing, ΔZ, as shown in Figure 2-1.

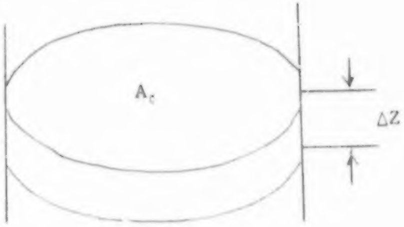

FIGURE 2-1 - DIFFERENTIAL HEIGHT OF PACKING

The number of moles, n_x, of HNO_x ($x = 2$ or 3) is given in Equation 2-1.

$$-dn_x = k_x a A_c P(y_x - y_x^*)dz \qquad (2\text{-}1)$$

For our column we assume that the equilibrium partial pressure over the liquid is zero. As a result of this assumption Equation 2-1 may be simplified.

$$-dn_x = k_x a A_c P y_x dz \qquad (2\text{-}2)$$

The moles of HNO_2 or HNO_3 transferred must be related to the NO and NO_2 removed from the gas. Radian's gas phase equilibrium model calculates y_x when given inputs of "chemical NO" and "chemical NO_2", C_{NO} and C_{NO_2}. From the reaction of NO and NO_2 to form HNO_2 and HNO_3 these relationships may be calculated.

$$H_2O + NO + NO_2 \rightarrow 2HNO_2 \qquad (2\text{-}3a)$$

$$H_2O + 2NO_2 \rightarrow HNO_2 + HNO_3 \qquad (2\text{-}3b)$$

$$dC_{NO} = \tfrac{1}{2}\left(dn_{HNO_2} - dn_{HNO_3}\right) \qquad (2\text{-}4a)$$

$$dC_{NO_2} = \tfrac{1}{2}\left(dn_{HNO_2} + 3dn_{HNO_3}\right) \qquad (2\text{-}4b)$$

If Equations 2-4a and b are combined with Equation 2-2. Equations 2-5a through 2-6b result, describing the decrease in total chemical NO and NO_2 as a function of the mass transfer of the molecular species HNO_2 and HNO_3.

$$-dC_{NO} = \tfrac{1}{2}\left(\alpha_1 y_{HNO_2} - \alpha_2 y_{HNO_3}\right)dz \qquad (2\text{-}5a)$$

$$-dC_{NO_2} = \tfrac{1}{2}\left(\alpha_1 y_{HNO_2} + 3\alpha_2 y_{HNO_3}\right)dz \qquad (2\text{-}5b)$$

$$\alpha_1 = k_{HNO_2} aPA_c \qquad (2\text{-}6a)$$

$$\alpha_2 = k_{HNO_3} aPA_c \qquad (2\text{-}6b)$$

Since y_{HNO_2} and y_{HNO_3} are complicated functions of C_{NO} and C_{NO_2} the equations must be integrated numerically.

The quantities that can be measured experimentally are total NO, C_{NO}, and total NO_2, C_{NO_2}. The quantities required in making mass transfer calculations are the mole fractions of HNO_2 and HNO_3. Values for both of these quantities are computed. Therefore, any error in the equilibrium constants that are used to compute y_{HNO_2} and y_{HNO_3} from the measured quantities C_{NO} and C_{NO_2} will show up as errors in k_ga values computed from experimental data. Thus, even if the mechanism has been correctly identified and the analytical chemistry measurements correctly made, the computed k_ga values may be incorrect in an absolute sense. Their use is justified so long as the same equilibrium constants used in calculating k_ga's are used in making mass transfer calculations with these k_ga's.

3.0 NUMERICAL CALCULATION SCHEME

Equation 2-5 may be integrated to give the amount removed in a packed column of height H.

$$-\left[C_{NO}\right]_{out} + \left[C_{NO}\right]_{in} = \tfrac{1}{2}\int_0^H \left(\alpha_1 y_{HNO_2} - \alpha_2 y_{HNO_3}\right)dz \qquad (3\text{-}1a)$$

$$-\left[C_{NO_2}\right]_{out} + \left[C_{NO_2}\right]_{in} = \tfrac{1}{2}\int_0^H \left(\alpha_1 y_{HNO_2} + 3\alpha_2 y_{HNO_3}\right)dz \qquad (3\text{-}1b)$$

Values of α_1 and α_2 are assumed. The right hand side of Equation 3-1 is numerically integrated. The error, ϕ, between the removal determined experimentally, rem, and that calculated is given in Equation 3-2.

$$\Phi_1 = \text{rem}_{NO} - \left(c_{in} - c_{out}\right)_{NO} \qquad (3\text{-}2a)$$

$$\Phi_2 = \text{rem}_{NO_2} - \left(c_{in} - c_{out}\right)_{NO_2} \qquad (3\text{-}2b)$$

The initial values for α_1 and α_2 will not yield the desired values of $\Phi_1 = \Phi_2 = 0$. A Newton-Raphson technique was used. This requires a knowledge of the derivatives of Equation 3-2.

$$\frac{\partial \Phi_1}{\partial \alpha_1} = \frac{1}{2} \int_0^H y_{HNO_2} dz \qquad (3\text{-}3a)$$

$$\frac{\partial \Phi_1}{\partial \alpha_2} = -\frac{1}{2} \int_0^H y_{HNO_3} dz \qquad (3\text{-}3b)$$

$$\frac{\partial \Phi_2}{\partial \alpha_1} = \frac{1}{2} \int_0^H y_{HNO_2} dz \qquad (3\text{-}3c)$$

$$\frac{\partial \Phi_2}{\partial \alpha_2} = \frac{3}{2} \int_0^H y_{HNO_3} dz \qquad (3\text{-}3d)$$

After the correct values of α_1 and α_2 have been chosen, the k_ga's may be calculated from Equation 2-6.

The experimental data used were those reported in T.N. 200-007-09. The data were recalculated to more accurately account for the amount removed. The actual amount of NO_x removed was accurately measured with liquid phase chemical analyses. This is shown below.

$$In_{gas} = Out_{gas} + Out_{liquid} \qquad (3\text{-}4)$$

The inlet and outlet gas concentrations were calculated as follows:

$$In_{avg} = \frac{In_{gas} + Out_{gas} + Out_{liquid}}{2} \qquad (3\text{-}5)$$

$$Out_{avg\ gas} = In_{avg} - Out_{liquid} \qquad (3\text{-}6)$$

This procedure maximized the accuracy of the difference between composition of gas_{in} and gas_{out} by making it equal to the accurately known liquid measurement. The original material balances are given in Table 3-1. The corrected gas compositions are given in Table 3-2.

4.0 RESULTS

Values of k_ga's for HNO_2 and HNO_3 were calculated from the equations given in Sections 2 and 3 and the data in Table 3-1. The results are given in Table 4-1.

The three points in Table 4-1 are plotted on log-log paper in Figure 4-1 for HNO_2 and Figure 4-2 for HNO_3. A slope of 0.8 was arbitrarily chosen for the vapor rate dependence. Since the data were all at one liquid rate, no correlation could be made. The liquid rate dependence was assumed to be 0.39 as reported by Brown* for NH_3. The following correlation is suggested for use within the constraints discussed above.

---

*Brown, G. G., Unit Operations, p. 530, John Wiley & Sons, New York, (1950).

TABLE 3-1
MATERIAL BALANCE SUMMARY
from TN 200-007-09

		Gas In (mole/min x 10^6)	Gas Out of Condenser	+	Scrubber Liquid Out (mole/min x 10^6)	+	Liquid Condensed	=	
Run 1	NO	102.76	97.54	+	21.14	+	?	=	118.68
	NO_2	101.03	52.84	+	60.08	+	?	=	112.92
Run 2	NO	135.6	134.05	+	21.72	+	(-3.2)	=	152.57
	NO_2	130.8	68.79	+	62.95	+	9	=	140.74
Run 3	NO	172.8	185.12	+	23.61	+	?	=	208.73
	NO_2	162.0	85.95	+	70.56	+	?	=	156.51

TABLE 3-2
CORRECTED MATERIAL BALANCE

		Gas In (mole/min x 10^6)	Gas Out (mole/min x 10^6)
Run 1	NO	110.72	89.58
	NO_2	106.97	46.89
Run 2	NO	144.10	122.38
	NO_2	135.75	72.80
Run 3	NO	190.75	167.14
	NO_2	159.25	88.69

TABLE 4-1

RESULTS OF MASS TRANSFER COEFFICIENT CALCULATIONS

Run No.	Vapor Flow Rate $\left[\frac{\text{normal } M^3}{\text{hour}}\right]$	Liquid Rate $\left[\frac{cm^3}{min}\right]$	$K_g a_{HNO_2}$ $\left[\frac{\text{gm mole}}{(hr)(cm^3)(atm)}\right]$	$K_g a_{HNO_3}$ $\left[\frac{\text{gm mole}}{(hr)(cm^3)(atm)}\right]$
1	0.728	710	0.277	0.972
2	0.948	710	0.275	0.962
3	1.18	710	0.302	1.22

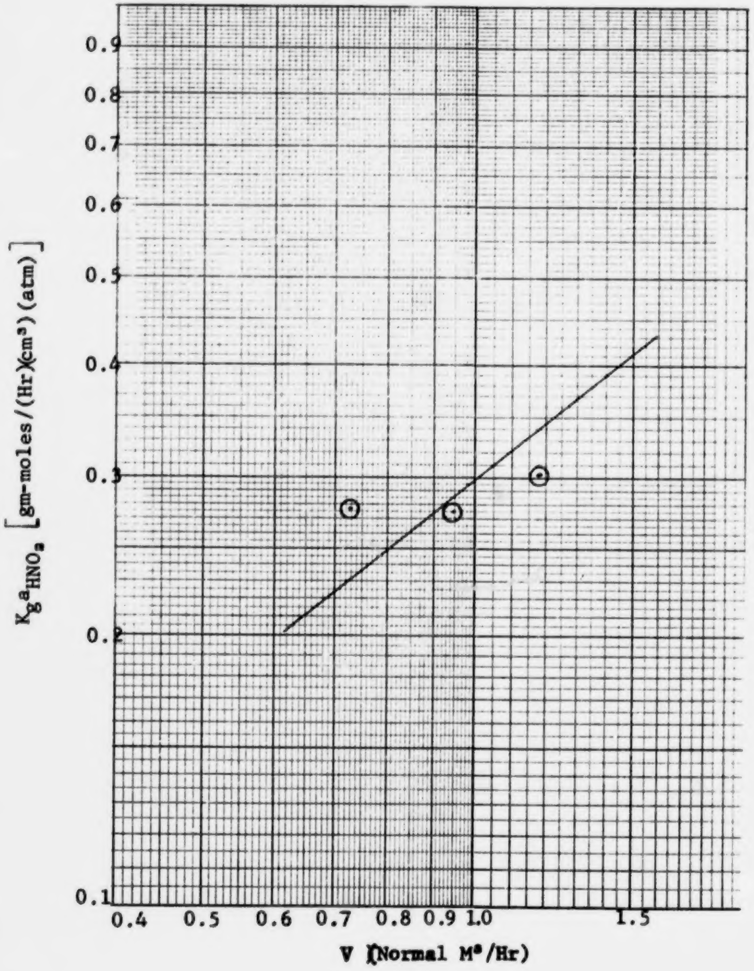

FIGURE 4-1

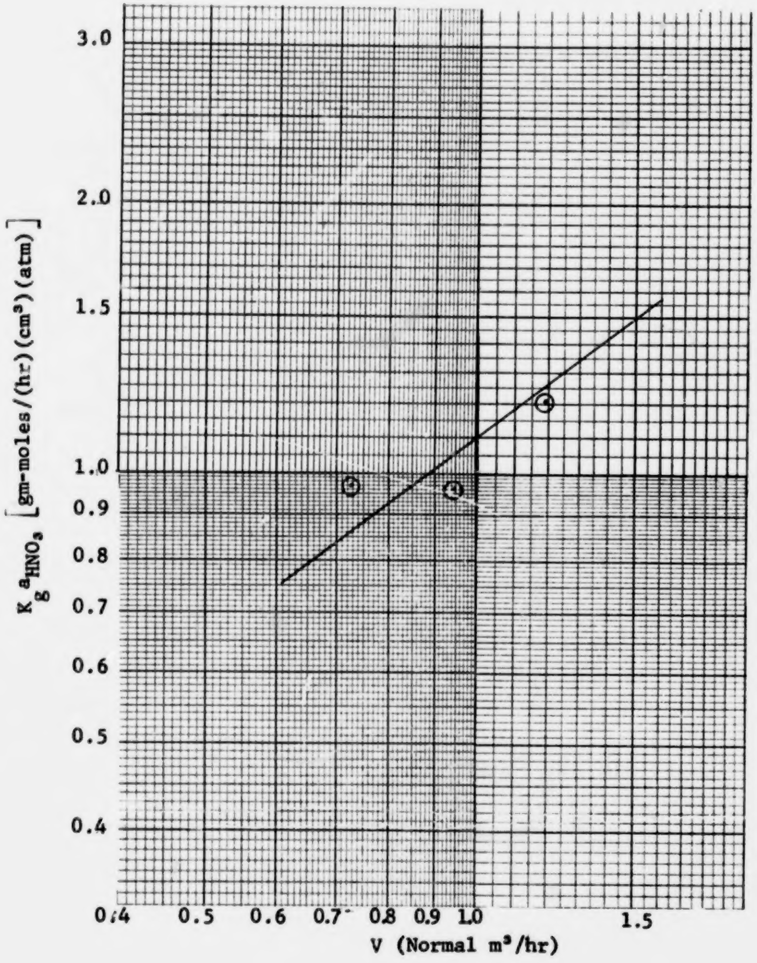

FIGURE 4-2

$$k_g a_{HNO_2} = 0.795 \left(\frac{V}{A}\right)_c^{0.8} \left(\frac{L}{A}\right)_c^{0.39} \qquad (4\text{-}1a)$$

$$k_g a_{HNO_3} = 2.96 \left(\frac{V}{A}\right)_c^{0.8} \left(\frac{L}{A}\right)_c^{0.39} \qquad (4\text{-}1b)$$

5.0 CONCLUSIONS

A mechanism has been proposed to explain mass transfer of NO and NO_2 from flue gases into aqueous alkaline solutions. It is based on gas film limited transfer of HNO_2 and HNO_3. Mass transfer coefficients have been calculated on the basis of this mechanism. These are given in Equations 4-1.

These equations and this mechanism must be considered as being tentative. The ratio of $k_g a_{HNO_2}/k_g a_{HNO_3}$ is 0.27 and not 1.04 as predicted by film theory. This might be due to inaccurate equilibrium constants used in calculating y_{HNO_2} or y_{HNO_3}. Not enough experimental data nor a large enough range of data were used in the correlation to give too much confidence in the results. On the other hand, these are the only data applicable to testing this specific hypothesis.

6.0 NOMENCLATURE

a	surface area of packing per volume of column (cm^2/cm^3)
A_c	crossectional area of column (cm^2)
C_{NO}, C_{NO_2}	chemical NO, chemical NO_2 (gmoles/min)
H	height of column (cm)
k	mass transfer coefficient (gmoles/hr cm^2 atm)
L	liquid rate (cm^3/min)
n	number of moles per hour
P	total pressure (atm)
rem	measured amount of HNO_2 or HNO_3 removal (gmoles/hr)
V	vapor rate (normal M^3/hr)
y	mole fraction in bulk gas
y*	mole fraction in gas in equilibrium with liquid
ΔZ	differential height of packing (cm)

Subscripts

x	x = 2 for HNO_2, x = 3 for HNO_3
1	HNO_2
2	HNO_3

Greek

ϕ	difference between measured and calculated amount of HNO_2 or HNO_3 removed (gmoles/hr)

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TECHNICAL NOTE 200-007-14

RESULTS OF LITERATURE SEARCH ON AQUEOUS SORPTION OF NITROGEN OXIDES

1 November 1971

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The object of the early data collection task was to define the problem by surveying all available literature on aqueous sorption of nitrogen oxides and associated subjects. There were four sources for acquisition of pertinent literature.

The first source was the bibliography in the final report, "Systems Study of Nitrogen Oxide Control Methods for Stationary Sources" prepared for NAPCA under Contract No. PH 22-68-55. Section 5.5.1 dealt with aqueous absorption of NO_x and the bibliography for that section gave thirteen pertinent references from which several other references of interest were found. In addition, the supplementary bibliography of 750 references was searched and nearly 100 titles were selected as applicable.

The second source of information was the Air Pollution Technical Information Center. NAPCA Publication AP-12, Nitrogen Oxides: An Annotated Bibliography was used. In addition the output from an APTIC computer search for information on nitrogen oxides and absorption was furnished by Tom Kittleman. About fifty abstracts of articles of interest were found. Some were duplicates of those from the first literature source.

The third source of information was the technical files at Radian. Some twenty references of interest were available through this source.

The fourth source of information was Chemical Abstracts. Cumulative indices from 1947 to 1966 were used as well as semi-annual indices for the period from 1967 to June, 1969. The biweekly issues from June, 1969, until October, 1970, were searched using the keyword index at the end of each issue. Abstracts which seemed useful were copied.

A file of abstracts from the four sources described above was assembled. As the program continued and new avenues of interest became evident, more literature was added to the data base. The abstracts were read and filed in the categories discussed below. A few references are listed in more than one category.

1. Mechanism of Absorption of Nitrogen Oxides by Aqueous Solutions and Chemistry of NO_x-H_2O Systems

The literature concerning NO_x-H_2O system chemistry and the mechanism of the reactions involved was reviewed in detail. It was used in preparing the problem definition for aqueous sorption (see Technical Note 200-007-01). Much of this literature is discussed in the review in Technical Note 200-007-02. Many interesting but not directly applicable references were not mentioned in the technical notes, although some were considered in detail. They are listed in part 1 of the supplementary bibliography at the end of this note.

2. Descriptions of and Operating Data for Aqueous Sorption Processes

The abstracts in this category were not investigated in detail. They are listed in part 2 of the supplementary bibliography.

3. NO_2-NO-H_2O Gas Phase Reactions and Kinetics Studies

References on homogeneous reaction equilibria in the gas phase were used in the problem definition for a computer program which calculates gas phase compositions in the $NO-NO_2-H_2O$ system. Additional references were used to verify resulting calculated equilibrium compositions. These are discussed in Technical Note 200-007-03a. Other references, including kinetic studies of both vapor phase and aqueous phase reactions have not been mentioned previously. These, and some of the ones used in the problem definition, are listed in part 3 of the supplemental bibliography.

4. Physical Properties and Thermodynamic Properties of Gaseous, Solid, and Aqueous Systems Containing Nitrogen Oxides or Oxyacids

This is a large, general category in which many abstracts were found. Some were useful for contract EHSD 71-5. Others were not pertinent then, but will be very useful for later work. Some of the abstracts in this category were further separated into more specific categories. These categories were:

- Thermodynamics of Electrolyte Solutions
- Solubility Data for Hydroxides, Nitrates and Nitrites
- Complex or Ion-Pair Formation Involving Nitrites, Nitrates, or Hydroxides
- Activity Coefficients and Equilibrium Constants.

These references are listed in part 4 of the supplemental bibliography.

5. Measured and Estimated Standard State Thermodynamic Properties of Solid Nitrates, Nitrites, Nitrides, and Hydroxides

These data are discussed in detail in Technical Note 200-007-04a and Technical Note 200-007-3a.

6. Thermal Analysis and Decomposition of Solid Nitrates and Nitrites

These references are given detailed consideration in Technical Note 200-007-06.

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TECHNICAL NOTE 200-007-15

CALCULATION OF DECOMPOSITION PRESSURES OVER METAL NITRATES AND NITRITES

9 December 1971

Prepared by:

Terry B. Parsons

Literature on the thermal stability of metal nitrites and nitrates has been reviewed in Technical Note 200-007-06. The data show that the salts decompose at relatively low temperatures, usually well below 700°C. The mechanism of the decompositions is quite complicated since the gaseous decomposition products and the melt interact.

Thermal decomposition of solid metal nitrates and nitrites was selected as a possible method of regenerating metal oxide sorbents for NO_x removal processes. In order to evaluate the effectiveness of several metal oxide sorbents, the relative free energies of the corresponding nitrate and nitrite thermal decomposition steps were investigated (see Technical Note 200-007-13).

The equilibrium constants and free energy changes for reactions such as (1) and (2), where Me stands for a metal, were calculated using standard state thermodynamic properties and heat capacities of products and reactants.

$$Me(NO_3)_2 \rightleftarrows MeO + N_2O_5 \quad (1)$$

$$Me(NO_2)_2 \rightleftarrows MeO + N_2O_3 \quad (2)$$

Thermodynamic data for reactions such as (3) and (4) were also investigated in order to describe decomposition in the presence of CO_2.

$$Me(NO_3)_2 + CO_2 \rightleftarrows MeCO_3 + N_2O_5 \quad (3)$$

$$Me(NO_2)_2 + CO_2 \rightleftarrows MeCO_3 + N_2O_3 \quad (4)$$

The results were calculated for the temperature range from 25 to 700°C. The changes in entropy and enthalpy and the logarithm of the equilibrium constant for the reactions were plotted versus temperature for reactions involving the metal nitrates and nitrites shown in Table I. The compounds which are marked by an asterisk are those for which calculations for reactions such as (3) and (4) were done. The results are given in the graphs and computer output on the following pages.

TABLE I

$AgNO_3$*
$AgNO_3$*
$Al(NO_3)_3$
$Ba(NO_3)_2$*
$Ba(NO_3)_2$*
$Be(NO_3)_2$
$Be(NO_3)_2$
$Bi(NO_3)_3$
$Ca(NO_3)_2$*
$Ca(NO_3)_2$*
$Cd(NO_3)$
$Cd(NO_3)_2$*
$Ce(NO_3)_4$
$Co(NO_3)_2$
$Co(NO_3)_2$
$CuNO_3$
$CuNO_3$
$Cu(NO_3)_2$
$Cu(NO_3)_2$
$Fe(NO_3)_3$
$Fe(NO_3)_3$
$Fe(NO_3)_3$

KNO_3*
KNO_3*
$LiNO_3$*
$LiNO_3$*
$Mg(NO_3)_2$
$Mg(NO_3)_2$*
$Mn(NO_3)_2$
$Mn(NO_3)_2$*
$Mn(NO_3)_3$
$NaNO_3$*
$NaNO_3$*
$Ni(NO_3)_2$
$Ni(NO_3)_2$
$Pb(NO_3)_2$*
$Pb(NO_3)_2$*
$Sn(NO_3)_4$
$Sr(NO_3)_2$*
$Sr(NO_3)_2$*
$Zn(NO_3)_2$
$Zn(NO_3)_2$
$Zr(NO_3)_4$*

```
SEPT.  1971                              2AGNO2  =  N2O3 + AG2O


    TEMPERATURE                ENTHALPY                ENTROPY                    LOG  K
      DEG. C                 CAL./GMOLE          CAL./GMOLE/DEG.K

     2.5000+01               3.4039+04               4.1704+01               -1.5835+01
     5.0000+01               3.4064+04               4.1783+01               -1.3905+01
     1.0000+02               3.4127+04               4.1966+01               -1.0815+01
     1.5000+02               3.4169+04               4.2072+01               -8.4521+00
     2.0000+02               3.4158+04               4.2047+01               -6.5874+00
     2.5000+02               3.4073+04               4.1879+01               -5.0811+00
     3.0000+02               3.3904+04               4.1571+01               -3.8422+00
      .5000+02               3.3640+04               4.1132+01               -2.8086+00
      .0000+02               3.3277+04               4.0572+01               -1.9368+00
      .5000+02               3.2810+04               3.9903+01               -1.1947+00
      .0000+02               3.2235+04               3.9136+01               -5.5884-01
      .5000+02               3.1551+04               3.8279+01               -1.0984-02
      .0000+02               3.0755+04               3.7340+01                4.6288-01
      .5000+02               2.9845+04               3.6328+01                8.7386-01
      .0000+02               2.8821+04               3.5248+01                1.2309+00
      .5000+02               2.7682+04               3.4108+01                1.5411+00

          HR PLOT COMPLETED
          SR PLOT COMPLETED
          LOG K PLOT COMPLETED
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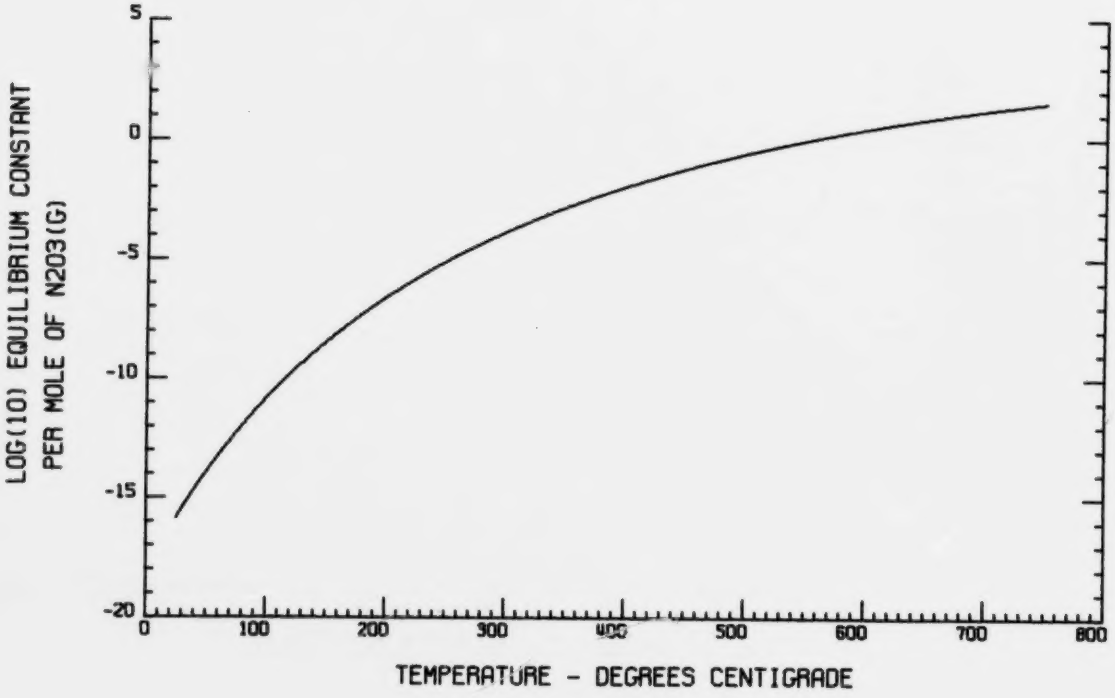
2AGNO2 = N2O3 + AG2O



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8  OCT.  1971                2AGNO2 + CO2 ❘ N2O3(G) + AG2CO3


      TEMPERATURE              ENTHALPY             ENTROPY                 LOG  K
       DEG. C                  CAL./GMOLE         CAL./GMOLE/DEG.K

      2.5000+01                1.4466+04            -2.2413+00             -1.1093+01
      5.0000+01                1.4554+04            -1.9588+00             -1.0270+01
      1.0000+02                1.4763+04            -1.3586+00             -8.9427+00
      1.5000+02                1.4975+04            -8.2425-01             -7.9140+00
      2.0000+02                1.5160+04            -4.1000-01             -7.0917+00
      2.5000+02                1.5300+04            -1.2945-01             -6.4194+00
      3.0000+02                1.5381+04             1.9940-02             -5.8602+00
      3.5000+02                1.5397+04             4.6892-02             -5.3892+00
      4.0000+02                1.5341+04            -3.7921-02             -4.9887+00
      4.5000+02                1.5211+04            -2.2388-01             -4.6457+00
      5.0000+02                1.5005+04            -5.0078-01             -4.3503+00
      5.5000+02                1.4717+04            -8.5948-01             -4.0950+00
      6.0000+02                1.4350+04            -1.2918+00             -3.8739+00
      6.5000+02                1.3902+04            -1.7904+00             -3.6822+00
      7.0000+02                1.3372+04            -2.3488+00             -3.5162+00
      7.5000+02                1.2760+04            -2.9613+00             -3.3727+00

          HR PLOT COMPLETED
          SR PLOT COMPLETED
          LOG K PLOT COMPLETED
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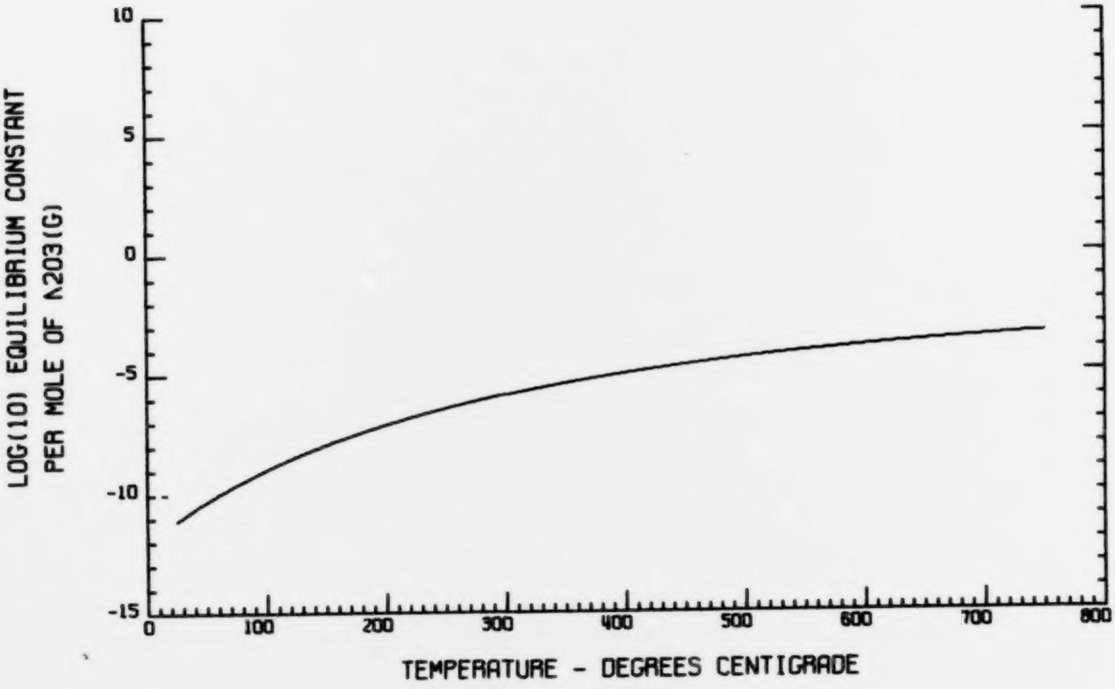
2AGNO2 + CO2 → N2O3(G) + AG2CO3



08 OCT 71

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10  AUG.  1971                    2AGNO3  =  N205 +AG20

                                                                              LOG  K
                                                       ENTROPY
   TEMPERATURE              ENTHALPY             CAL./GMOLE/DEG.K
     DEG. C                CAL./GMOLE
                                                                          -3.0482+01
   2.5000+01               5.4859+04               4.4514+01              -2.6848+01
   5.0000+01               6.8220+04               8.8253+01              -2.0687+01
   1.0000+02               6.7727+04               8.6835+01              -1.6019+01
   1.5000+02               6.7159+04               8.5409+01              -1.2427+01
   2.0000+02               6.5154+04               8.0835+01              -9.7584+00
   2.5000+02               5.8880+04               6.7894+01              -7.6252+00
   3.0000+02               5.6188+04               6.6629+01              -5.8546+00
   3.5000+02               5.7551+04               6.5563+01              -4.3631+00
   4.0000+02               5.6961+04               6.4653+01              -3.0906+00
   4.5000+02               5.6414+04               6.3868+01              -1.9930+00
   5.0000+02               5.5903+04               6.3185+01              -1.0372+00
   5.5000+02               5.5427+04               6.2588+01              -1.9796-01
   6.0000+02               5.4983+04               6.2064+01               5.4459-01
   6.5000+02               5.4568+04               6.1602+01               1.2060+00
   7.0000+02               5.4181+04               6.1193+01               1.7986+00
   7.5000+02               5.3821+04               6.0833+01

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        SR PLOT COMPLETED
        LOG K PLOT COMPLETED
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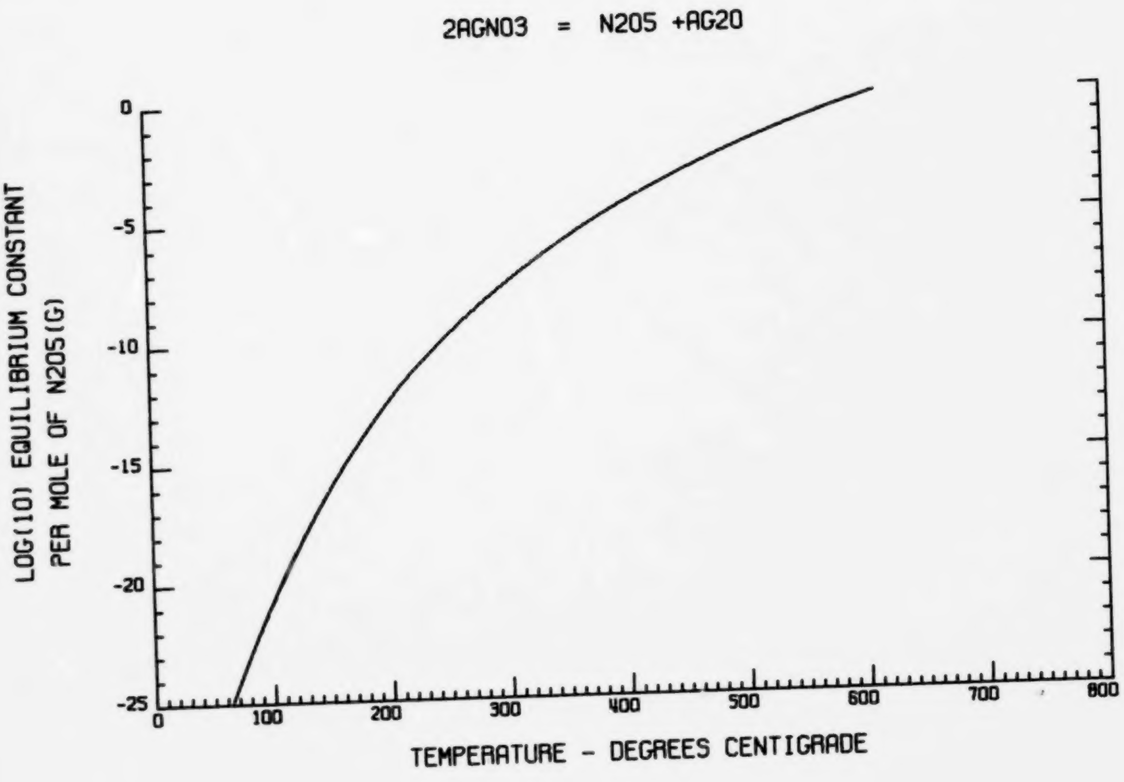

10 AUG 71

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8  OCT.  1971                 2AGNO3 + CO2 I N2O5(G) + AG2CO3


    TEMPERATURE            ENTHALPY               ENTROPY              LOG  K
     DEG. C               CAL./GMOLE         CAL./GMOLE/DEG.K

    2.5000+01             3.5286+04             5.6871-01           -2.5739+01
    5.0000+01             4.8710+04             4.4511+01           -2.3213+01
    1.0000+02             4.8363+04             4.3511+01           -1.8814+01
    1.5000+02             4.7965+04             4.2513+01           -1.5481+01
    2.0000+02             4.6157+04             3.8378+01           -1.2932+01
    2.5000+02             4.0106+04             2.5885+01           -1.1097+01
    3.0000+02             3.9665+04             2.5078+01           -9.6432+00
    3.5000+02             3.9307+04             2.4479+01           -8.4352+00
    4.0000+02             3.9025+04             2.4043+01           -7.4151+00
    4.5000+02             3.8815+04             2.3741+01           -6.5415+00
    5.0000+02             3.8672+04             2.3549+01           -5.7844+00
    5.5000+02             3.8593+04             2.3450+01           -5.1212+00
    6.0000+02             3.8578+04             2.3432+01           -4.5347+00
    6.5000+02             3.8624+04             2.3483+01           -4.0115+00
    7.0000+02             3.8732+04             2.3596+01           -3.5411+00
    7.5000+02             3.8899+04             2.3764+01           -3.1152+00

         HR PLOT COMPLETED
         SR PLOT COMPLETED
         LOG K PLOT COMPLETED
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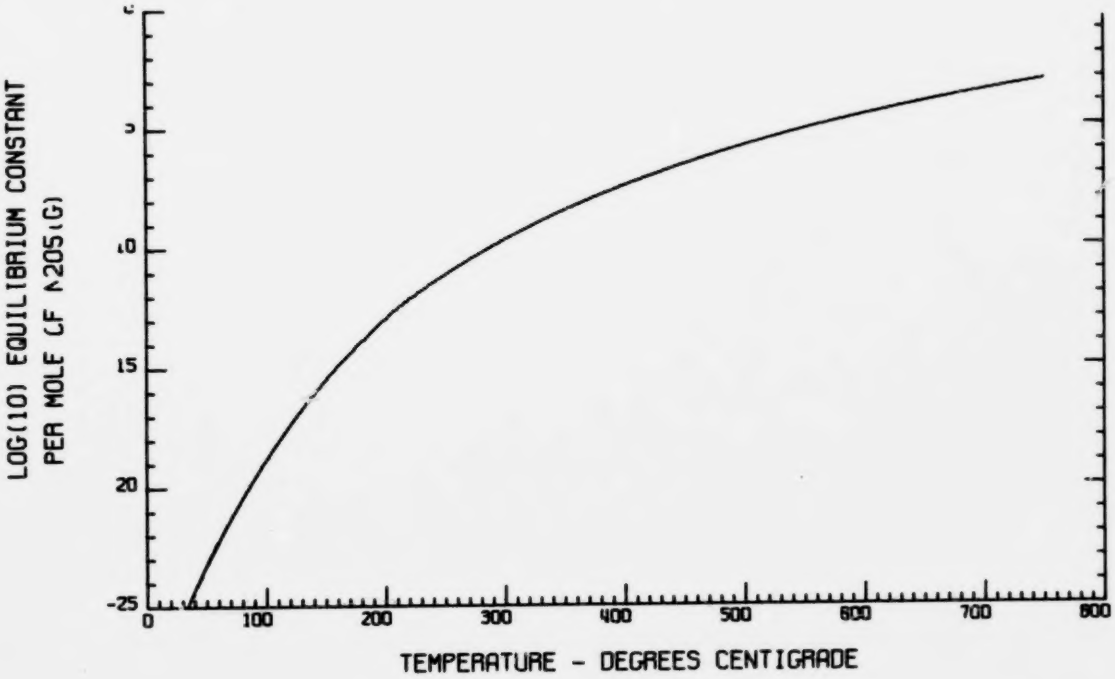
2AGNO3 + CO2 → N2O5(G) + AG2CO3



08 OCT 71

```
9 SEPT.  1971                         2AL(NO3)3  =  3N205 + AL203

                                                                                  LOG  K
      TEMPERATURE            ENTHALPY                 ENTROPY
        DEG. C             CAL./GMOLE          CAL./GMOLE/DEG.K

       2.5000+01            2.8901+04              5.1523+01             -9.9233+00
       5.0000+01            4.2339+04              9.5511+01             -7.7593+00
       1.0000+02            4.2010+04              9.4565+01             -3.9369+00
       1.5000+02            4.1664+04              9.3695+01             -1.0412+00
       2.0000+02            4.1293+04              9.2867+01              1.2230+00
       2.5000+02            4.0893+04              9.2063+01              3.0374+00
       3.0000+02            4.0460+04              9.1274+01              4.5200+00
       3.5000+02            3.9994+04              9.0495+01              5.7510+00
       4.0000+02            3.9492+04              8.9720+01              6.7865+00
       4.5000+02            3.8953+04              8.8949+01              7.6671+00
       5.0000+02            3.8378+04              8.8179+01              8.4229+00
       5.5000+02            3.7764+04              8.7411+01              9.0768+00
       6.0000+02            3.7112+04              8.6642+01              9.6461+00
       6.5000+02            3.6422+04              8.5874+01              1.0145+01
       7.0000+02            3.5693+04              8.5105+01              1.0583+01
       7.5000+02            3.4924+04              8.4335+01              1.0971+01

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          LOG K PLOT COMPLETED
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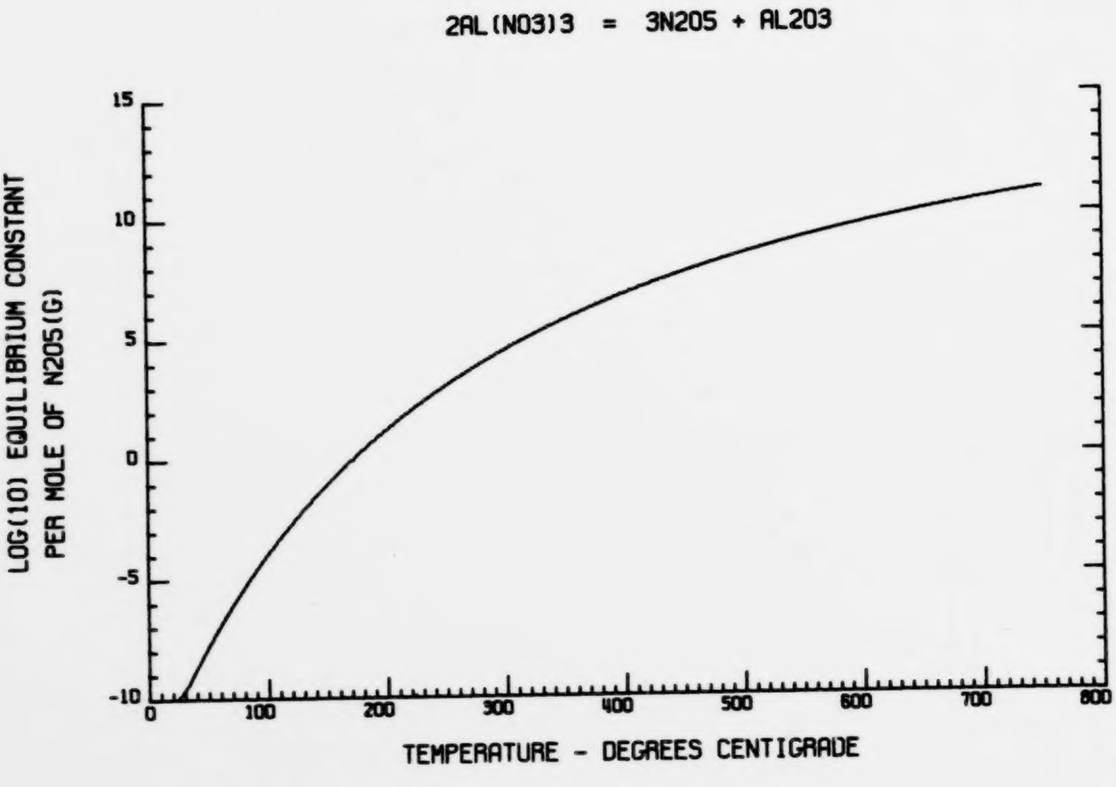


09 SEP 71

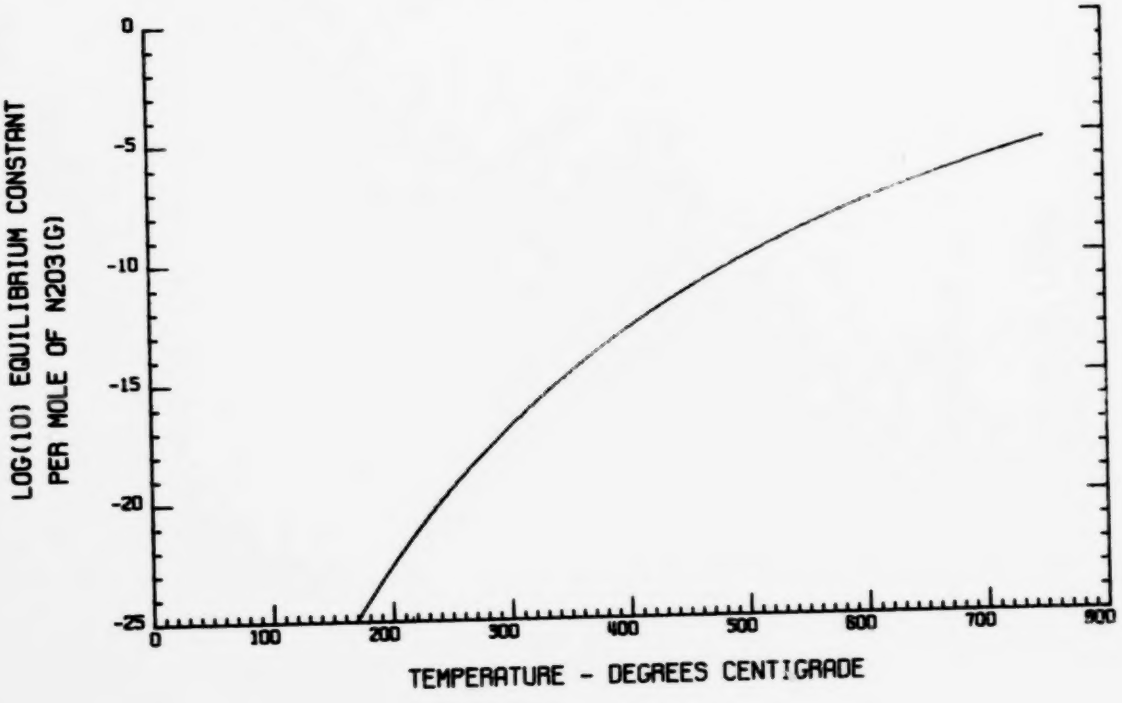
```
9 SEPT.  1971                      BA(NO2)2  =  N2O3(G) + BAO

  TEMPERATURE           ENTHALPY              ENTROPY              LOG  K
   DEG. C             CAL./GMOLE       CAL./GMOLE/DEG.K

  2.5000+01           7.1327+04           4.7005+01           -4.2007+01
  5.0000+01           7.1351+04           4.7083+01           -3.7962+01
  1.0000+02           7.1415+04           4.7267+01           -3.1494+01
  1.5000+02           7.1456+04           4.7372+01           -2.6551+01
  2.0000+02           7.1445+04           4.7348+01           -2.2651+01
  2.5000+02           7.1361+04           4.7180+01           -1.9499+01
  3.0000+02           7.1191+04           4.6871+01           -1.6901+01
  3.5000+02           7.0928+04           4.6432+01           -1.4727+01
  4.0000+02           7.0565+04           4.5872+01           -1.2884+01
  4.5000+02           7.0097+04           4.5204+01           -1.1305+01
  5.0000+02           6.9523+04           4.4436+01           -9.9401+00
  5.5000+02           6.8838+04           4.3579+01           -8.7520+00
  6.0000+02           6.8042+04           4.2640+01           -7.7113+00
  6.5000+02           6.7133+04           4.1628+01           -6.7949+00
  7.0000+02           6.6109+04           4.0549+01           -5.9844+00
  7.5000+02           6.4970+04           3.9408+01           -5.2649+00

        HR PLOT COMPLETED
        SR PLOT COMPLETED
        LOG K PLOT COMPLETED
```

BA(NO2)2 = N2O3(G) + BAO



09 SEP 71

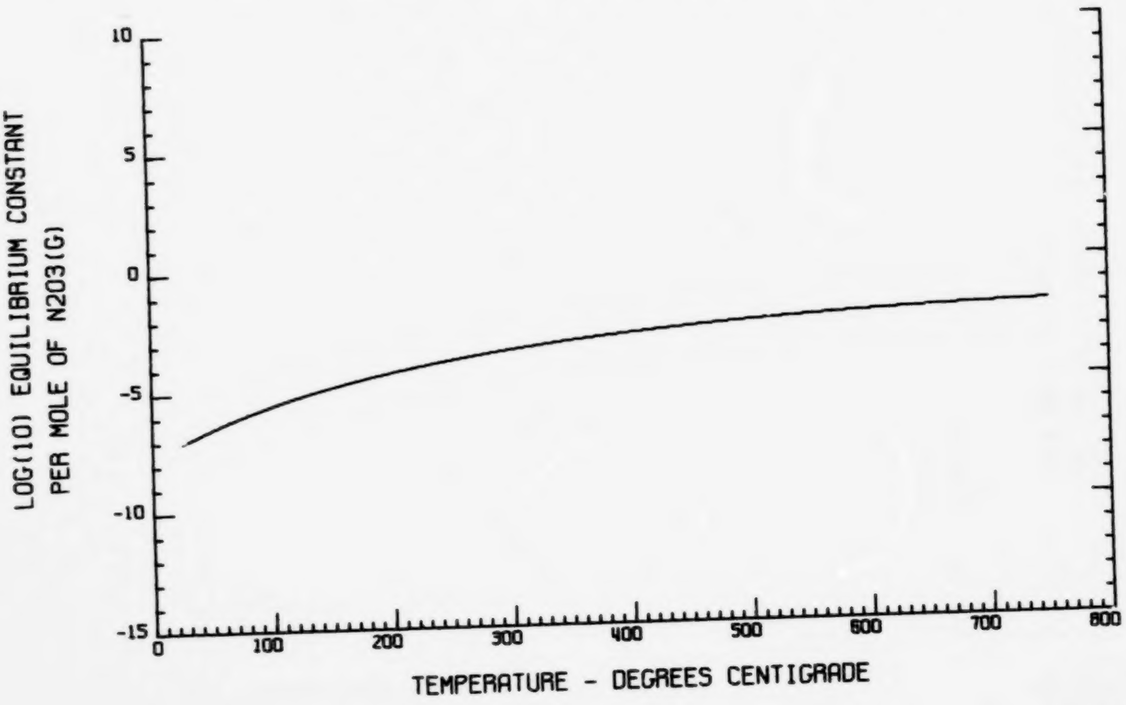
```
8 OCT. 1971                 BA(NO2)2 + CO2  I  N2O3(G) + BACO3

                                                                          LOG  K
   TEMPERATURE              ENTHALPY                  ENTROPY
     DEG. C                CAL./GMOLE            CAL./GMOLE/DEG.K

    2.5000+01              1.0252+04                2.1514+00           -7.0459+00
    5.0000+01              1.0258+04                2.1718+00           -6.4626+00
    1.0000+02              1.0321+04                2.3510+00           -5.5307+00
    1.5000+02              1.0398+04                2.5446+00           -4.8139+00
    2.0000+02              1.0450+04                2.6607+00           -4.2449+00
    2.5000+02              1.0452+04                2.6665+00           -3.7854+00
    3.0000+02              1.0390+04                2.5537+00           -3.4054+00
    3.5000+02              1.0252+04                2.3251+00           -3.0874+00
    4.0000+02              1.0033+04                1.9876+00           -2.8229+00
    4.5000+02              9.7273+03                1.5498+00           -2.6009+00
    5.0000+02              9.3310+03                1.0206+00           -2.4144+00
    5.5000+02              8.8420+03                4.0836-01           -2.2582+00
    6.0000+02              8.2585+03               -2.7925-01           -2.1280+00
    6.5000+02              7.5793+03               -1.0352+00           -2.0205+00
    7.0000+02              6.8056+03               -1.8530+00           -1.9328+00
    7.5000+02              5.9308+03               -2.7272+00           -1.8628+00

          HR PLOT COMPLETED
          SR PLOT COMPLETED
          LOG K PLOT COMPLETED
```

BA(NO2)2 + CO2 - N2O3(G) + BACO3



08 OCT 71

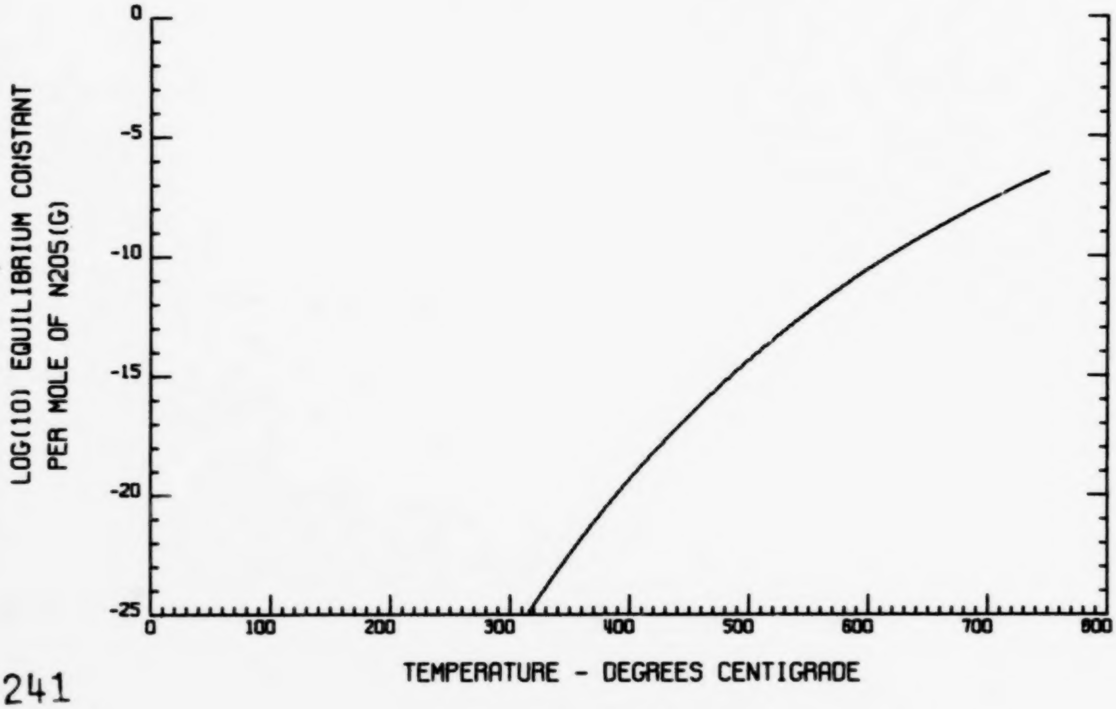
```
10  AUG.  1971                          BA(NO3)2  =  N205(G) + BAO

        TEMPERATURE                ENTHALPY                 ENTROPY                    LOG  K
          DEG. C                 CAL./GMOLE           CAL./GMOLE/DEG.K

        2.5000+01               1.0774+05                4.8495+01                 -6.8369+01
        5.0000+01               1.2120+05                9.2567+01                 -6.1734+01
        1.0000+02               1.2099+05                9.1947+01                 -5.0761+01
        1.5000+02               1.2060+05                9.1473+01                 -4.2395+01
        2.0000+02               1.2060+05                9.1034+01                 -3.5808+01
        2.5000+02               1.2037+05                9.0578+01                 -3.0489+01
        3.0000+02               1.2010+05                9.0082+01                 -2.6107+01
        3.5000+02               1.1978+05                8.9537+01                 -2.2437+01
        4.0000+02               1.1939+05                8.8940+01                 -1.9322+01
        4.5000+02               1.1894+05                8.8292+01                 -1.6647+01
        5.0000+02               1.1841+05                8.7593+01                 -1.4326+01
        5.5000+02               1.1782+05                8.6848+01                 -1.2300+01
        6.0000+02               1.1115+05                7.9146+01                 -1.0522+01
        6.5000+02               1.1040+05                7.8318+01                 -9.0201+00
        7.0000+02               1.0958+05                7.7450+01                 -7.6821+00
        7.5000+02               1.0868+05                7.6547+01                 -6.4844+00

            HR PLOT COMPLETED
            SR PLOT COMPLETED
            LOG K PLOT COMPLETED
```

BA(NO3)2 = N205(G) + BAO



10 AUG 71

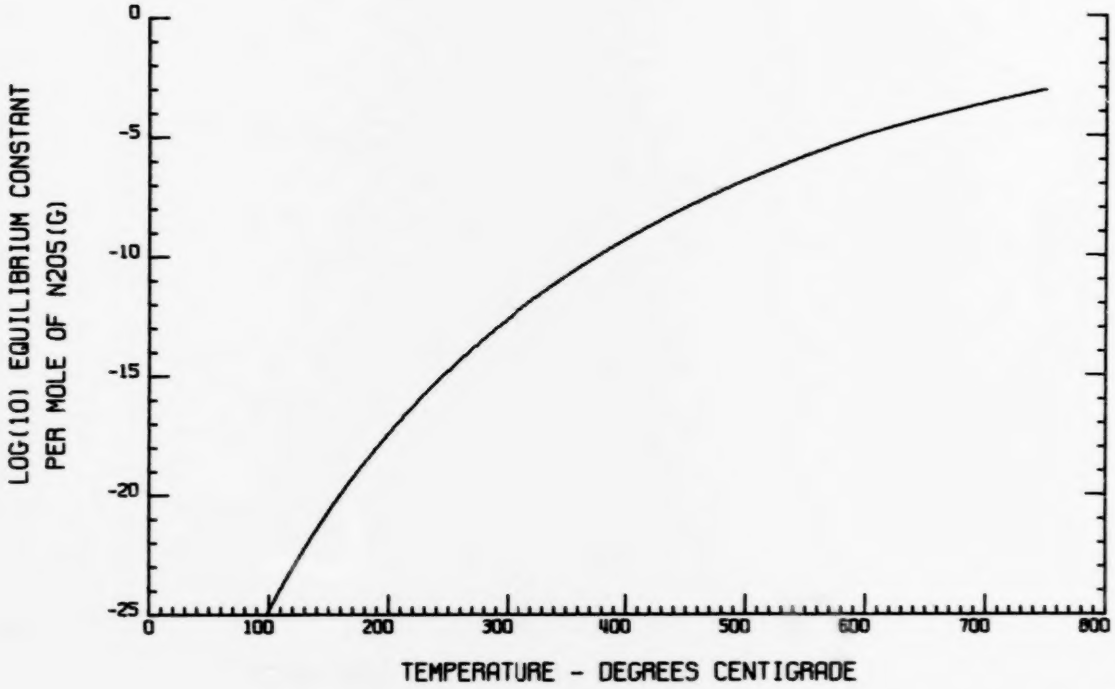
```
8  OCT.  1971                    BA(NO3)2 + CO2  I  N2O5 + BACO3


        TEMPERATURE              ENTHALPY                ENTROPY                  LOG  K
         DEG. C                CAL./GMOLE          CAL./GMOLE/DEG.K

        2.5000+01              4.6662+04              3.6414+00              -3.3405+01
        5.0000+01              6.0109+04              4.7656+01              -3.0234+01
        1.0000+02              5.9893+04              4.7031+01              -2.4798+01
        1.5000+02              5.9740+04              4.6645+01              -2.0658+01
        2.0000+02              5.9606+04              4.6347+01              -1.7402+01
        2.5000+02              5.9465+04              4.6065+01              -1.4774+01
        3.0000+02              5.9301+04              4.5764+01              -1.2609+01
        3.5000+02              5.9101+04              4.5430+01              -1.0798+01
        4.0000+02              5.8858+04              4.5055+01              -9.2616+00
        4.5000+02              5.8566+04              4.4638+01              -7.9435+00
        5.0000+02              5.8221+04              4.4178+01              -6.8022+00
        5.5000+02              5.7822+04              4.3677+01              -5.8058+00
        6.0000+02              5.1365+04              3.6228+01              -4.9388+00
        6.5000+02              5.0850+04              3.5654+01              -4.2458+00
        7.0000+02              5.0275+04              3.5048+01              -3.6307+00
        7.5000+02              4.9640+04              3.4412+01              -3.0824+00

            HR PLOT COMPLETED
            SR PLOT COMPLETED
            LOG K PLOT COMPLETED
```

BA(NO3)2 + CO2 - N2O5 + BACO3



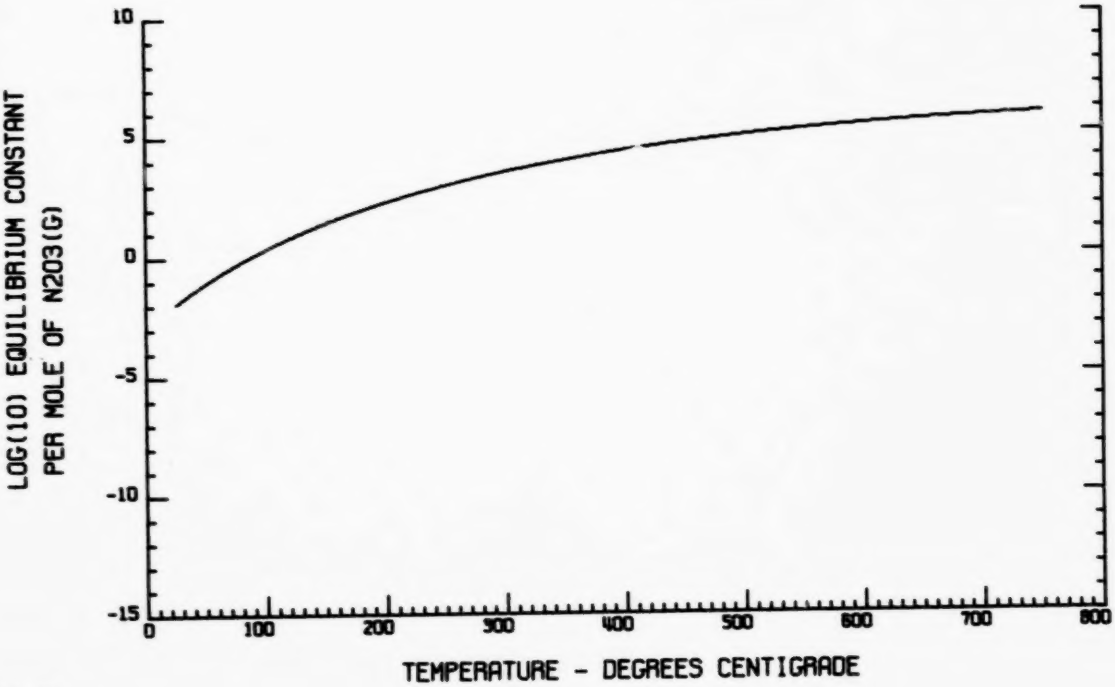
```
9 SEPT.  1971                    BE(NO2)2  =  N2O3(G) + BEO


      TEMPERATURE            ENTHALPY              ENTROPY              LOG  K
       DEG. C              CAL./GMOLE          CAL./GMOLE/DEG.K

      2.5000+01            1.5421+04             4.2978+01            -1.9102+00
      5.0000+01            1.5445+04             4.3057+01            -1.0352+00
      1.0000+02            1.5509+04             4.3240+01             3.6709-01
      1.5000+02            1.5550+04             4.3346+01             1.4419+00
      2.0000+02            1.5539+04             4.3321+01             2.2905+00
      2.5000+02            1.5454+04             4.3153+01             2.9749+00
      3.0000+02            1.5285+04             4.2845+01             3.5354+00
      3.5000+02            1.5021+04             4.2405+01             3.9993+00
      4.0000+02            1.4658+04             4.1846+01             4.3862+00
      4.5000+02            1.4191+04             4.1177+01             4.7103+00
      5.0000+02            1.3616+04             4.0409+01             4.9823+00
      5.5000+02            1.2932+04             3.9552+01             5.2105+00
      6.0000+02            1.2135+04             3.8614+01             5.4013+00
      6.5000+02            1.1226+04             3.7601+01             5.5599+00
      7.0000+02            1.0202+04             3.6522+01             5.6904+00
      7.5000+02            9.0630+03             3.5381+01             5.7963+00

           HR PLOT COMPLETED
           SR PLOT COMPLETED
           LOG K PLOT COMPLETED
```

BE(NO2)2 = N2O3(G) + BEO



09 SEP 71

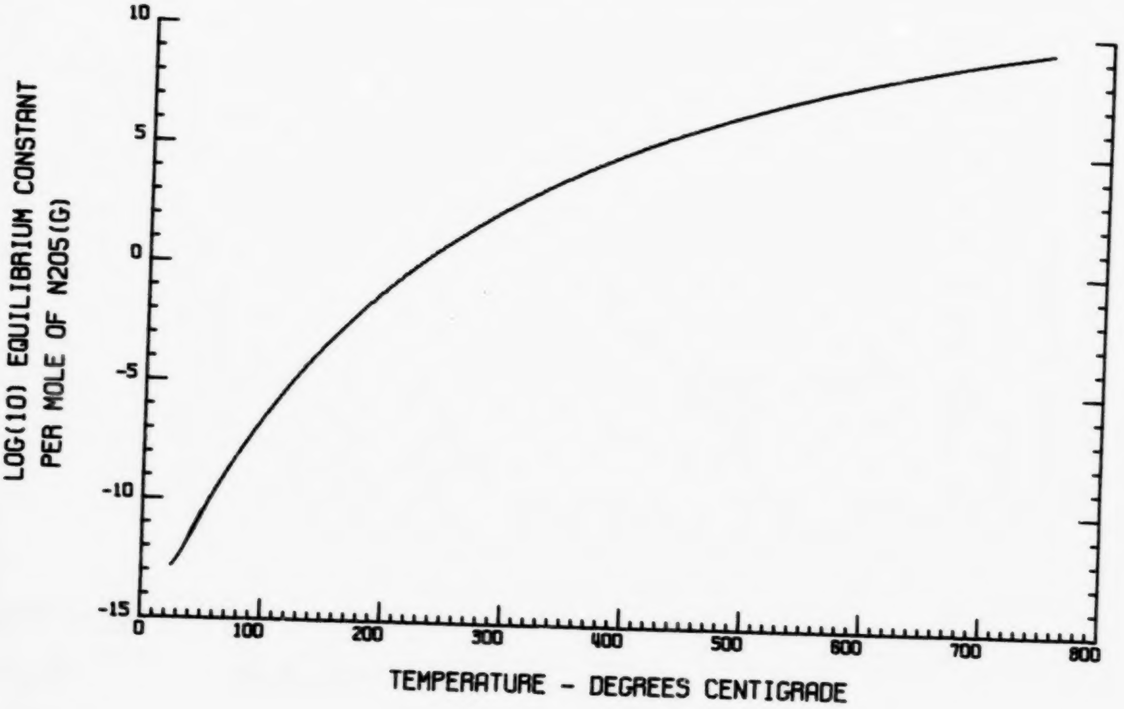
```
9 SEPT.  1971                         BE(NO3)2  =  N2O5(G) +BEO

   TEMPERATURE            ENTHALPY              ENTROPY                    LOG  K
    DEG. C               CAL./GMOLE         CAL./GMOLE/DEG.K

   2.5000+01             3.1381+04
   5.0000+01             4.4819+04            4.6568+01              -1.2824+01
   1.0000+02             4.4490+04            9.0557+01              -1.0519+01
   1.5000+02             4.4144+04            8.9612+01              -6.4719+00
   2.0000+02             4.3773+04            8.8741+01              -3.4046+00
   2.5000+02             4.3373+04            8.7913+01              -1.0051+00
   3.0000+02             4.2941+04            8.7110+01               9.1875-01
   3.5000+02             4.2475+04            8.6321+01               2.4918+00
   4.0000+02             4.1973+04            8.5542+01               3.7986+00
   4.5000+02             4.1434+04            8.4768+01               4.8987+00
   5.0000+02             4.0859+04            8.3996+01               5.8350+00
   5.5000+02             4.0245+04            8.3227+01               6.6394+00
   6.0000+02             3.9594+04            8.2458+01               7.3358+00
   6.5000+02             3.8903+04            8.1690+01               7.9428+00
   7.0000+02             3.8174+04            8.0922+01               8.4750+00
   7.5000+02             3.7406+04            8.0153+01               8.9438+00
                                              7.9383+01               9.3586+00

       HR PLOT COMPLETED
       SR PLOT COMPLETED
       LOG K PLOT COMPLETED
```

BE(NO3)2 = N2O5(G) +BEO



09 SEP 71

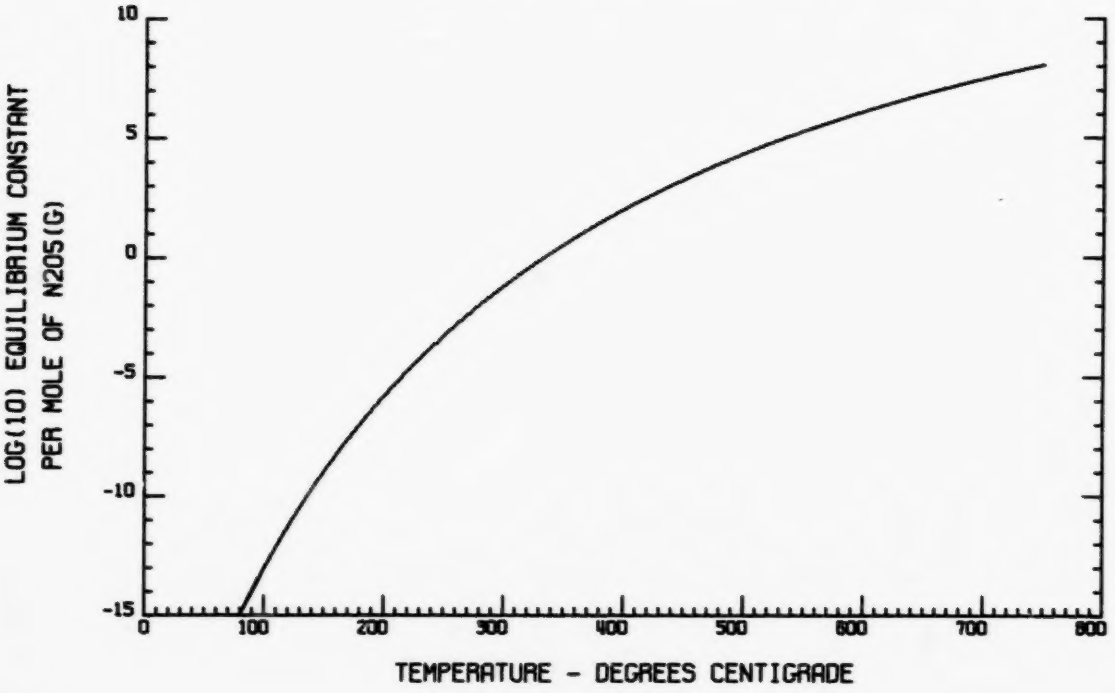
```
9 SEPT.  1971                    2BI(NO3)3  =  3N205(G) + BI203

    TEMPERATURE              ENTHALPY              ENTROPY                LOG  K
     DEG. C                 CAL./GMOLE        CAL./GMOLE/DEG.K

     2.5000+01              4.5479+04             5.4441+01            -2.1437+01
     5.0000+01              5.8917+04             9.8429+01            -1.8333+01
     1.0000+02              5.8588+04             9.7483+01            -1.3008+01
     1.5000+02              5.8242+04             9.6612+01            -8.9652+00
     2.0000+02              5.7871+04             9.5784+01            -5.7963+00
     2.5000+02              5.7471+04             9.4980+01            -3.2502+00
     3.0000+02              5.7038+04             9.4192+01            -1.1634+00
     3.5000+02              5.6572+04             9.3412+01             5.7471-01
     4.0000+02              5.6070+04             9.2637+01             2.0420+00
     4.5000+02              5.5531+04             9.1866+01             3.2947+00
     5.0000+02              5.4955+04             9.1096+01             4.3746+00
     5.5000+02              5.4342+04             9.0327+01             5.3130+00
     6.0000+02              5.3690+04             8.9559+01             6.1343+00
     6.5000+02              5.2999+04             8.8790+01             6.8576+00
     7.0000+02              5.2270+04             8.8021+01             7.4979+00
     7.5000+02              5.1502+04             8.7251+01             8.0674+00

          HR PLOT COMPLETED
          SR PLOT COMPLETED
          LOG K PLOT COMPLETED
```

2BI(NO3)3 = 3N205(G) + BI203



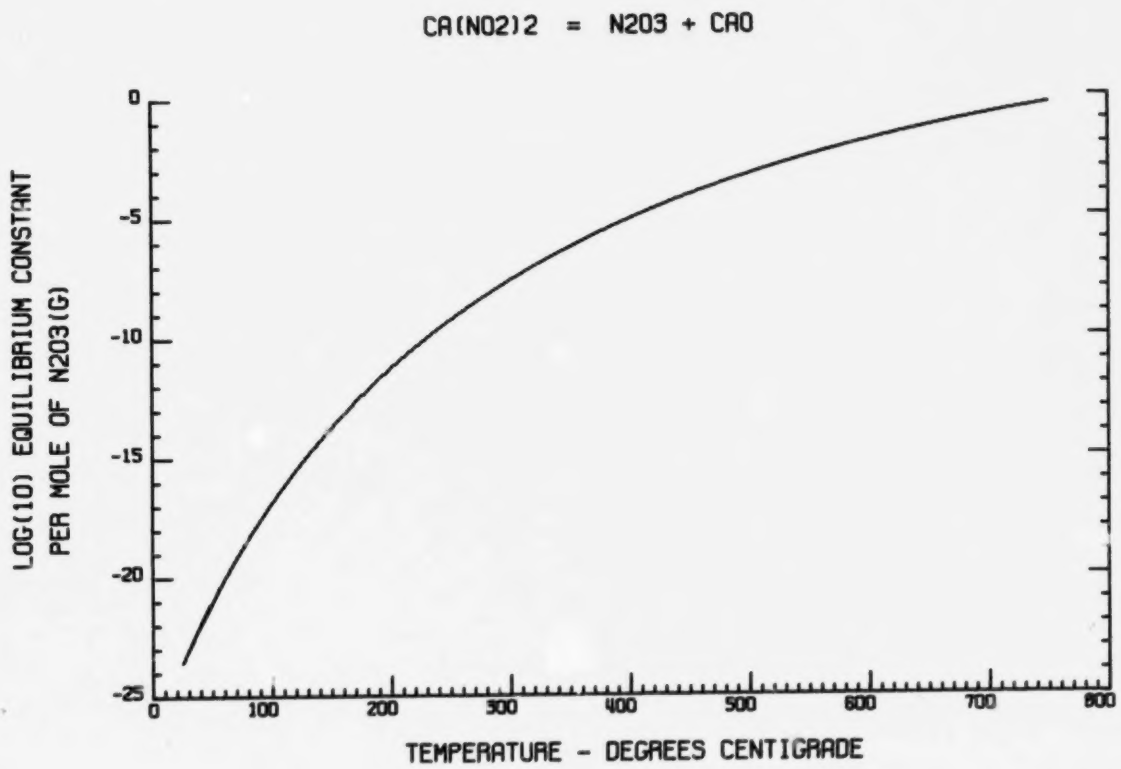
09 SEP 71

```
9 SEPT.  1971                    CA(NO2)2  =  N2O3 + CAO

    TEMPERATURE             ENTHALPY              ENTROPY                 LOG  K
     DEG. C               CAL./GMOLE        CAL./GMOLE/DEG.K

     2.5000+01             4.5275+04             4.4094+01             -2.3548+01
     5.0000+01             4.5299+04             4.4173+01             -2.0980+01
     1.0000+02             4.5363+04             4.4356+01             -1.6873+01
     1.5000+02             4.5404+04             4.4462+01             -1.3732+01
     2.0000+02             4.5393+04             4.4437+01             -1.1254+01
     2.5000+02             4.5309+04             4.4270+01             -9.2521+00
     3.0000+02             4.5139+04             4.3961+01             -7.6037+00
     3.5000+02             4.4876+04             4.3522+01             -6.2264+00
     4.0000+02             4.4513+04             4.2962+01             -5.0619+00
     4.5000+02             4.4045+04             4.2294+01             -4.0677+00
     5.0000+02             4.3471+04             4.1526+01             -3.2122+00
     5.5000+02             4.2786+04             4.0669+01             -2.4714+00
     6.0000+02             4.1990+04             3.9731+01             -1.8268+00
     6.5000+02             4.1081+04             3.8719+01             -1.2635+00
     7.0000+02             4.0057+04             3.7639+01             -7.6981-01
     7.5000+02             3.8918+04             3.6498+01             -3.3625-01

          HR PLOT COMPLETED
          SR PLOT COMPLETED
          LOG K PLOT COMPLETED
```



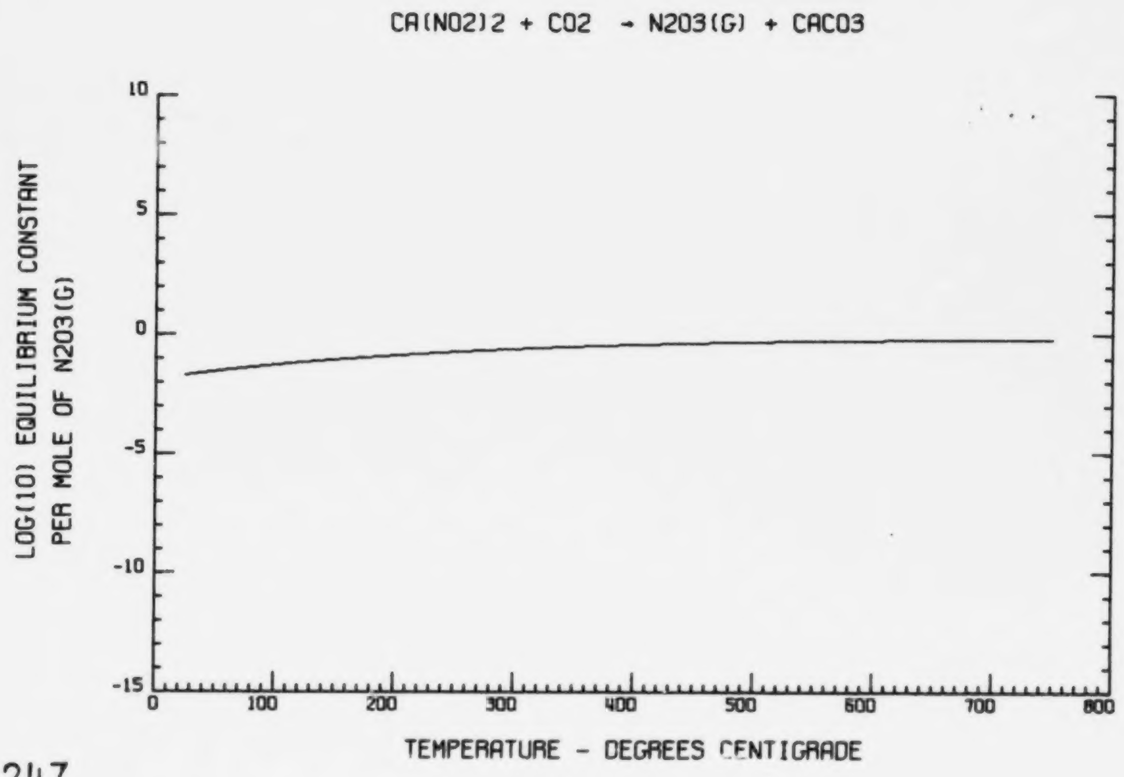
09 SEP 71

```
8  OCT.  1971                    CA(NO2)2 + CO2  I N203(G) + CACO3

     TEMPERATURE               ENTHALPY              ENTROPY                  LOG  K
      DEG. C                  CAL./GMOLE       CAL./GMOLE/DEG.K

     2.5000+01                2.8961+03            1.9646+00              -1.6934+00
     5.0000+01                2.9338+03            2.0853+00              -1.5283+00
     1.0000+02                3.0651+03            2.4613+00              -1.2571+00
     1.5000+02                3.2113+03            2.8293+00              -1.0401+00
     2.0000+02                3.3277+03            3.0903+00              -8.6163-01
     2.5000+02                3.3870+03            3.2106+00              -7.1322-01
     3.0000+02                3.3716+03            3.1834+00              -5.8983-01
     3.5000+02                3.2696+03            3.0139+00              -4.8797-01
     4.0000+02                3.0731+03            2.7116+00              -4.0509-01
     4.5000+02                2.7764+03            2.2873+00              -3.3917-01
     5.0000+02                2.3755+03            1.7520+00              -2.8857-01
     5.5000+02                1.8675+03            1.1160+00              -2.5191-01
     6.0000+02                1.2504+03            3.8884-01              -2.2798-01
     6.5000+02                5.2265+02           -4.2107-01              -2.1575-01
     7.0000+02               -3.1674+02           -1.3961+00              -2.1430-01
     7.5000+02               -1.2685+03           -2.2[illegible]93+00              -2.2281-01

         HR PLOT COMPLETED
         SR PLOT COMPLETED
         LOG K PLOT COMPLETED
```



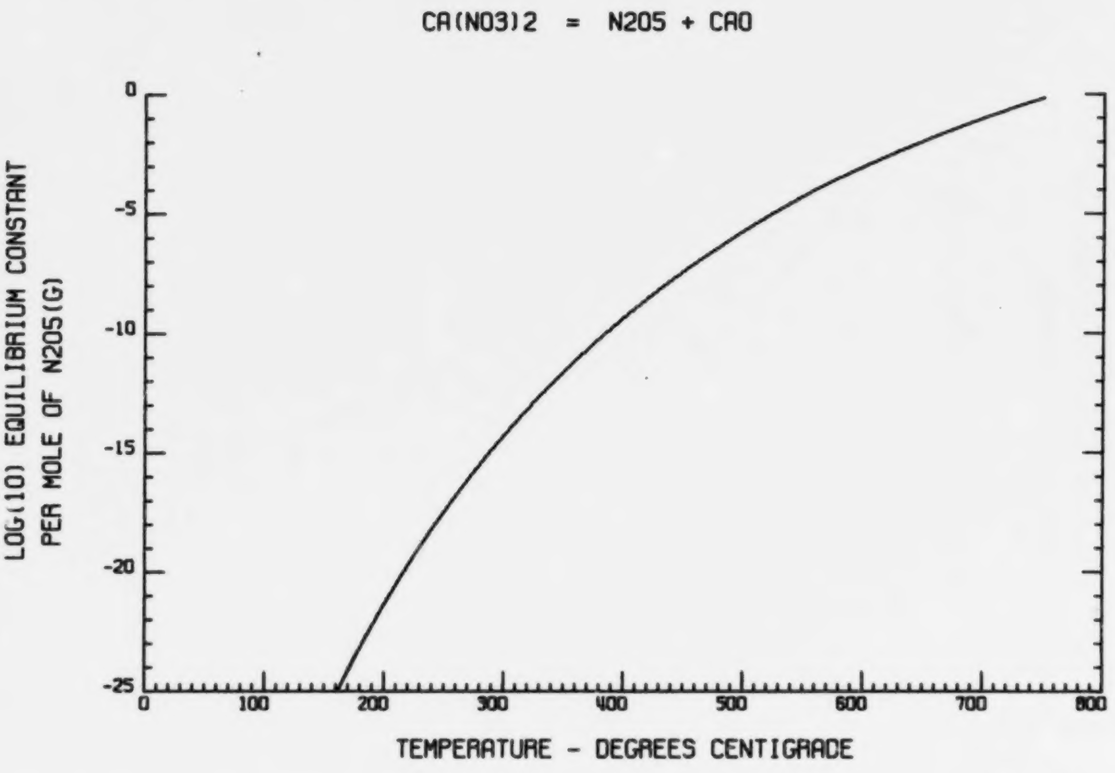
08 OCT 71

```
10  AUG.  1971                    CA(NO3)2  =  N205 + CAO

     TEMPERATURE            ENTHALPY              ENTROPY                 LOG  K
      DEG. C               CAL./GMOLE         CAL./GMOLE/DEG.K

      2.5000+01            7.5255+04             4.6084+01             -4.5087+01
      5.0000+01            8.8718+04             9.0152+01             -4.0294+01
      1.0000+02            8.8493+04             8.9502+01             -3.2266+01
      1.5000+02            8.8287+04             8.8986+01             -2.6149+01
      2.0000+02            8.8066+04             8.8496+01             -2.1336+01
      2.5000+02            8.7613+04             8.7984+01             -1.7454+01
      3.0000+02            8.7509+04             8.7431+01             -1.4259+01
      3.5000+02            8.7148+04             8.6827+01             -1.1587+01
      4.0000+02            8.6721+04             8.6169+01             -9.3225+00
      4.5000+02            8.6226+04             8.5459+01             -7.3812+00
      5.0000+02            8.5657+04             8.4700+01             -5.7014+00
      5.5000+02            8.5013+04             8.3893+01             -4.2360+00
      6.0000+02            7.9201+04             7.6940+01             -3.0085+00
      6.5000+02            7.8401+04             7.6049+01             -1.9400+00
      7.0000+02            7.7520+04             7.5120+01             -9.9165-01
      7.5000+02            7.6557+04             7.4156+01             -1.4605-01

         HR PLOT COMPLETED
         SR PLOT COMPLETED
         LOG K PLOT COMPLETED
```

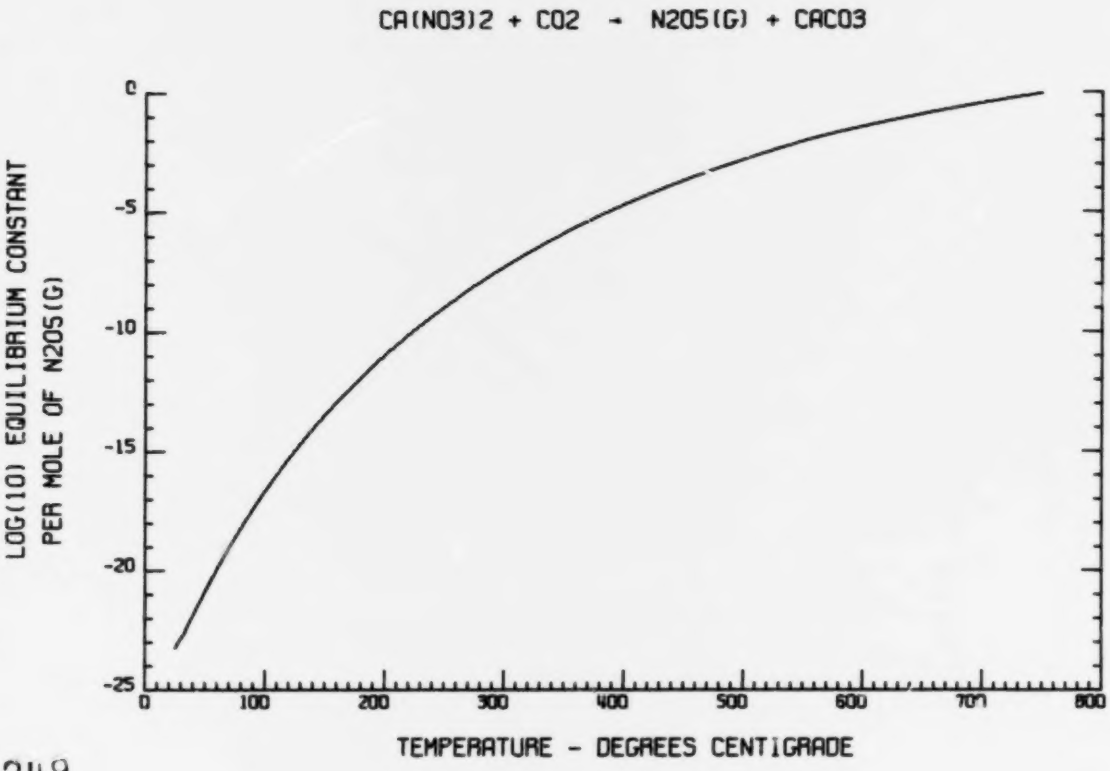


```
8  OCT.  1971                    CA(NO3)2 + CO2  I  N2O5(G) + CACO3

    TEMPERATURE              ENTHALPY              ENTROPY                 LOG  K
     DEG. C                 CAL./GMOLE         CAL./GMOLE/DEG.K

    2.5000+01              3.2876+04             3.9546+00             -2.3233+01
    5.0000+01              4.6352+04             4.8064+01             -2.0842+01
    1.0000+02              4.6195+04             4.7607+01             -1.6650+01
    1.5000+02              4.6094+04             4.7353+01             -1.3457+01
    2.0000+02              4.6002+04             4.7148+01             -1.0943+01
    2.5000+02              4.5891+04             4.6925+01             -8.9151+00
    3.0000+02              4.5742+04             4.6653+01             -7.2453+00
    3.5000+02              4.5541+04             4.6318+01             -5.8487+00
    4.0000+02              4.5281+04             4.5918+01             -4.6656+00
    4.5000+02              4.4956+04             4.5453+01             -3.6526+00
    5.0000+02              4.4562+04             4.4925+01             -2.7777+00
    5.5000+02              4.4094+04             4.4340+01             -2.0165+00
    6.0000+02              3.8461+04             3.7598+01             -1.4096+00
    6.5000+02              3.7842+04             3.6909+01             -8.9229-01
    7.0000+02              3.7146+04             3.6175+01             -4.3610-01
    7.5000+02              3.6370+04             3.5398+01             -3.2577-02

         HR PLOT COMPLETED
         SR PLOT COMPLETED
         LOG K PLOT COMPLETED
```



08 OCT 71

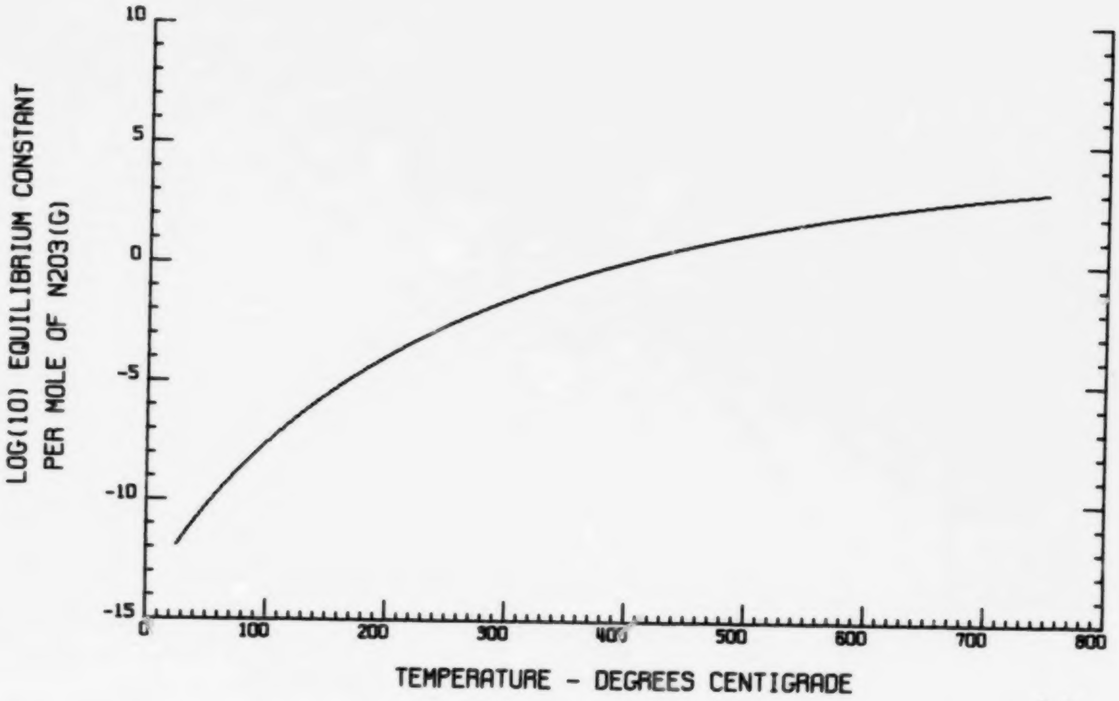
```
9 SEPT.  1971                          CD(NO2)2  =  N2O3 + CDO

      TEMPERATURE            ENTHALPY              ENTROPY                 LOG  K
       DEG. C               CAL./GMOLE        CAL./GMOLE/DEG.K

      2.5000+01             2.9388+04            4.4102+01             -1.1902+01
      5.0000+01             2.9412+04            4.4180+01             -1.0235+01
      1.0000+02             2.9476+04            4.4363+01             -7.5672+00
      1.5000+02             2.9517+04            4.4469+01             -5.5259+00
      2.0000+02             2.9506+04            4.4444+01             -3.9150+00
      2.5000+02             2.9421+04            4.4276+01             -2.6141+00
      3.0000+02             2.9252+04            4.3968+01             -1.5447+00
      3.5000+02             2.8988+04            4.3528+01             -6.5344-01
      4.0000+02             2.8625+04            4.2969+01              9.7280-02
      4.5000+02             2.8158+04            4.2300+01              7.3489-01
      5.0000+02             2.7583+04            4.1532+01              1.2799+00
      5.5000+02             2.6899+04            4.0675+01              1.7478+00
      6.0000+02             2.6102+04            3.9737+01              2.1510+00
      6.5000+02             2.5193+04            3.8724+01              2.4989+00
      7.0000+02             2.4169+04            3.7645+01              2.7993+00
      7.5000+02             2.3030+04            3.6504+01              3.0585+00

          HR PLOT COMPLETED
          SR PLOT COMPLETED
          LOG K PLOT COMPLETED
```

CD(NO2)2 = N2O3 + CDO



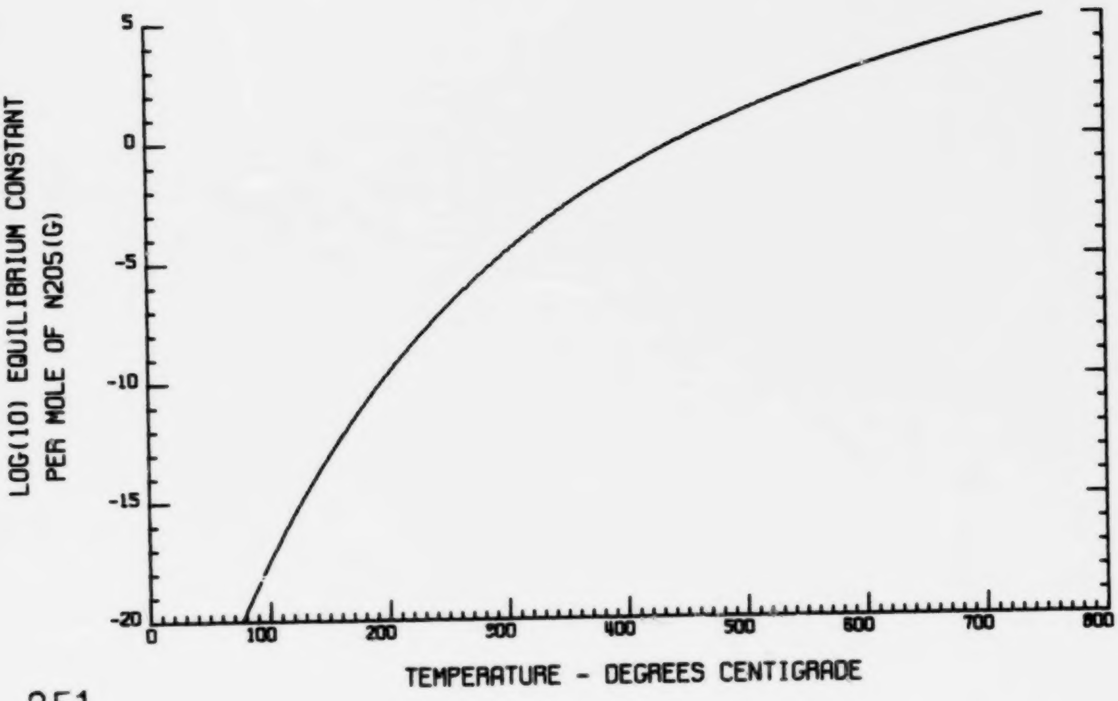
```
9 SEPT.  1971                      CD(NO3)2  =  N2O5 + CDO

     TEMPERATURE           ENTHALPY             ENTROPY              LOG  K
       DEG. C            CAL./GMOLE      CAL./GMOLE/DEG.K

     2.5000+01           5.0578+04           4.7692+01          -2.6649+01
     5.0000+01           6.4016+04           9.1680+01          -2.3256+01
     1.0000+02           6.3687+04           9.0734+01          -1.7469+01
     1.5000+02           6.3341+04           8.9864+01          -1.5073+01
     2.0000+02           6.2970+04           8.9036+01          -9.6263+00
     2.5000+02           6.2570+04           8.8232+01          -6.8551+00
     3.0000+02           6.2137+04           8.7443+01          -4.5825+00
     3.5000+02           6.1671+04           8.6664+01          -2.6884+00
     4.0000+02           5.6821+04           7.9022+01          -1.1774+00
     4.5000+02           5.6283+04           7.8251+01           9.2212-02
     5.0000+02           5.5707+04           7.7481+01           1.1867+00
     5.5000+02           5.5094+04           7.6713+01           2.1381+00
     6.0000+02           5.4442+04           7.5944+01           2.9708+00
     6.5000+02           5.3751+04           7.5176+01           3.7043+00
     7.0000+02           5.3022+04           7.4407+01           4.3537+00
     7.5000+02           5.2254+04           7.3637+01           4.9315+00

            HR PLOT COMPLETED
            SR PLOT COMPLETED
            LOG K PLOT COMPLETED
```

CD(NO3)2 = N2O5 + CDO



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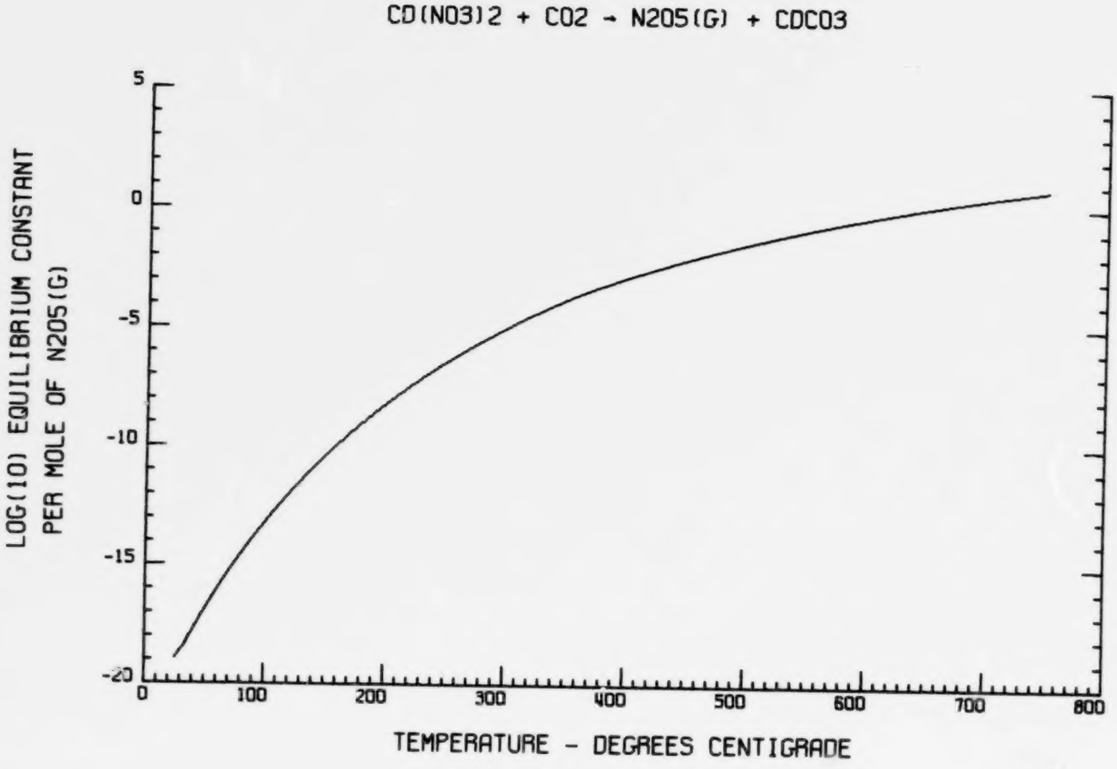
```
8  OCT.  1971                 CD(NO3)2 + CO2 I N2O5(G) + CDCO3

     TEMPERATURE            ENTHALPY               ENTROPY                  LOG  K
      DEG. C              CAL./GMOLE         CAL./GMOLE/DEG.K

     2.5000+01            2.7311+04             4.9408+00              -1.8958+01
     5.0000+01            4.0743+04             4.8906+01              -1.6865+01
     1.0000+02            4.0457+04             4.8084+01              -1.5186+01
     1.5000+02            4.0206+04             4.7456+01              -1.0394+01
     2.0000+02            3.9970+04             4.6924+01              -8.2063+00
     2.5000+02            3.9728+04             4.6438+01              -6.4471+00
     3.0000+02            3.9474+04             4.5974+01              -5.0038+00
     3.5000+02            3.9200+04             4.5516+01              -3.8002+00
     4.0000+02            3.4554+04             3.8190+01              -2.8720+00
     4.5000+02            3.4251+04             3.7727+01              -2.0998+00
     5.0000+02            3.3879+04             3.7257+01              -1.4342+00
     5.5000+02            3.3498+04             3.6779+01              -8.5564-01
     6.0000+02            3.3087+04             3.6294+01              -3.4940-01
     6.5000+02            3.2644+04             3.5802+01               9.6216-02
     7.0000+02            3.2171+04             3.5303+01               4.9047-01
     7.5000+02            3.1666+04             3.4797+01               8.4083-01

          HR PLOT COMPLETED
          SR PLOT COMPLETED
          LOG K PLOT COMPLETED
```

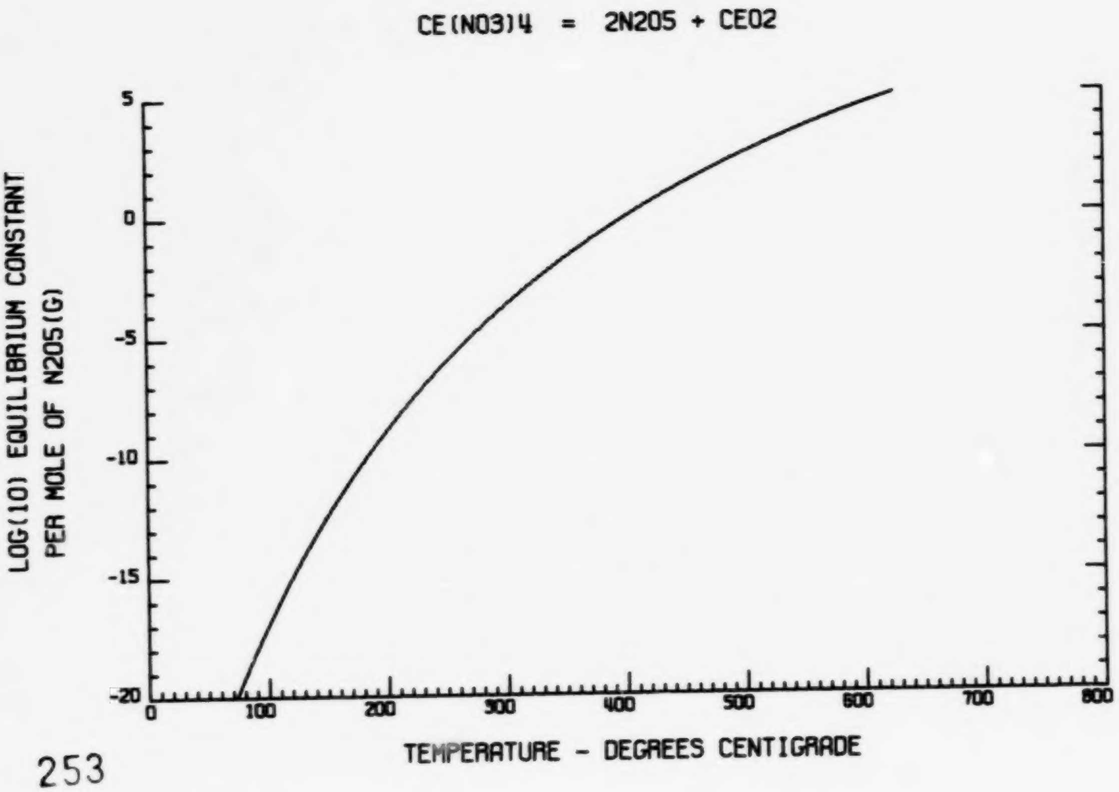


```
9 SEPT.  1971                         CE(NO3)4  =  2N205 + CE02


   TEMPERATURE            ENTHALPY              ENTROPY              LOG  K
    DEG. C              CAL./GMOLE        CAL./GMOLE/DEG.K

   2.5000+01            5.2530+04           5.5345+01           -2.6407+01
   5.0000+01            6.5968+04           9.9333+01           -2.2903+01
   1.0000+02            6.5640+04           9.8387+01           -1.6940+01
   1.5000+02            6.5293+04           9.7517+01           -1.2409+01
   2.0000+02            6.4922+04           9.6689+01           -8.8555+00
   2.5000+02            6.4522+04           9.5885+01           -5.9981+00
   3.0000+02            6.4090+04           9.5096+01           -3.6544+00
   3.5000+02            6.3623+04           9.4316+01           -1.7005+00
   4.0000+02            6.3121+04           9.3542+01           -4.9553-02
   4.5000+02            6.2583+04           9.2770+01            1.3615+00
   5.0000+02            6.2007+04           9.2001+01            2.5791+00
   5.5000+02            6.1393+04           9.1232+01            3.6386+00
   6.0000+02            6.0741+04           9.0463+01            4.5671+00
   6.5000+02            6.0051+04           8.9694+01            5.3860+00
   7.0000+02            5.9321+04           8.8925+01            6.1120+00
   7.5000+02            5.8553+04           8.8155+01            6.7589+00

         HR PLOT COMPLETED
         SR PLOT COMPLETED
         LOG K PLOT COMPLETED
```



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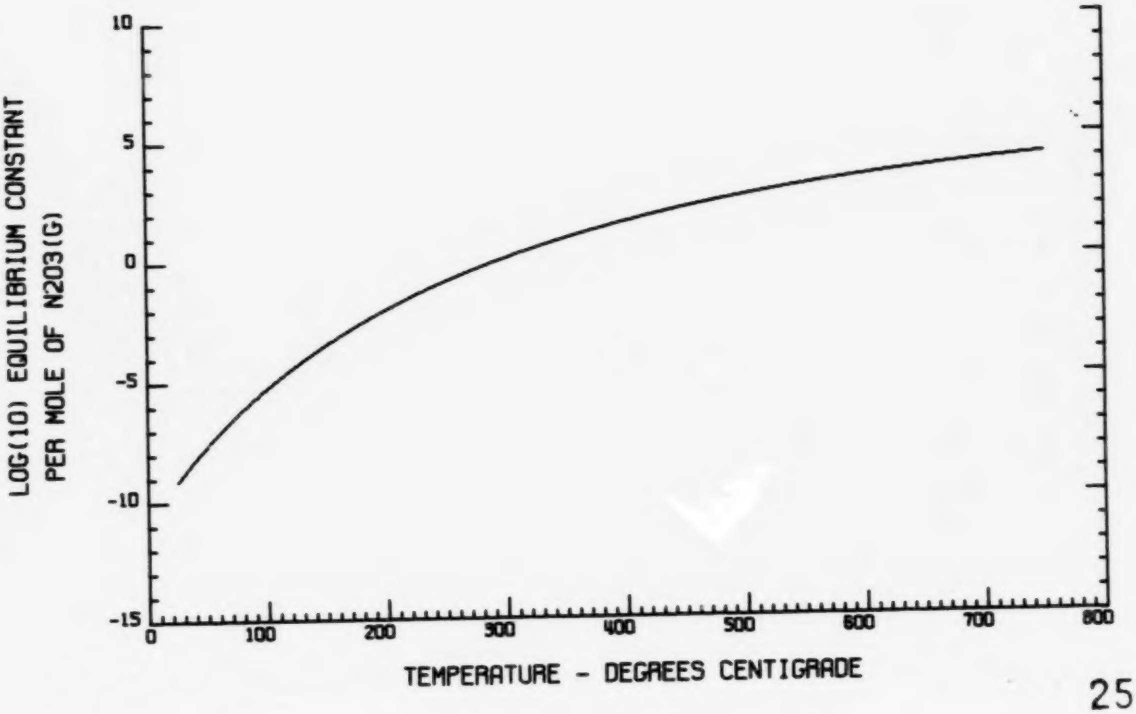
```
9 SEPT.  1971                       CO(NO2)2  =  N2O3 + COO

                                                                         LOG  K
  TEMPERATURE            ENTHALPY               ENTROPY
   DEG. C               CAL./GMOLE         CAL./GMOLE/DEG.K

                                                                      -9.1048+00
  2.5000+01             2.6127+04             4.5965+01              -7.6228+00
  5.0000+01             2.6151+04             4.6043+01              -5.2504+00
  1.0000+02             2.6215+04             4.6226+01              -3.4347+00
  1.5000+02             2.6257+04             4.6332+01              -2.0018+00
  2.0000+02             2.6245+04             4.6308+01              -8.4477-01
  2.5000+02             2.6161+04             4.6140+01               1.0585-01
  3.0000+02             2.5991+04             4.5831+01               8.9731-01
  3.5000+02             2.5728+04             4.5392+01               1.5631+00
  4.0000+02             2.5365+04             4.4833+01               2.1275+00
  4.5000+02             2.4897+04             4.4164+01               2.6088+00
  5.0000+02             2.4323+04             4.3396+01               3.0208+00
  5.5000+02             2.3638+04             4.2539+01               3.3744+00
  6.0000+02             2.2842+04             4.1601+01               3.6781+00
  6.5000+02             2.1933+04             4.0589+01               3.9389+00
  7.0000+02             2.0909+04             3.9509+01               4.1625+00
  7.5000+02             1.9770+04             3.8368+01

        HR PLOT COMPLETED
        SR PLOT COMPLETED
        LOG K PLOT COMPLETED
```

CO(NO2)2 = N2O3 + COO



09 SEP 71

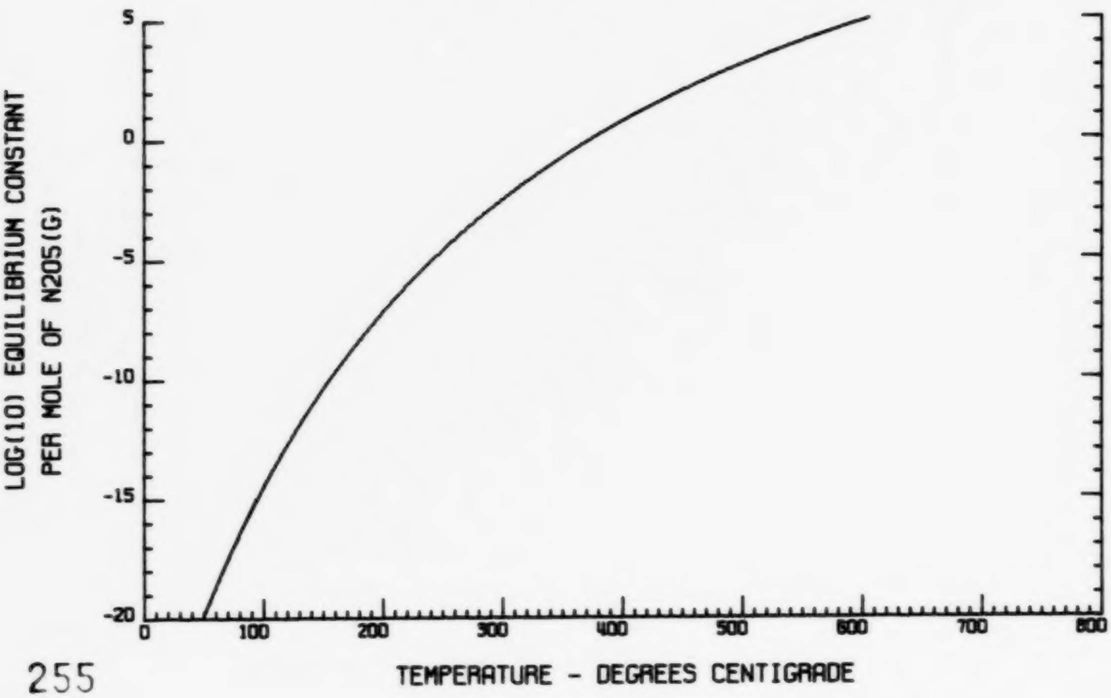
```
9 SEPT.  1971                          CO(NO3)2  =  N2O5 + COO


     TEMPERATURE              ENTHALPY                ENTROPY                 LOG  K
      DEG. C                 CAL./GMOLE           CAL./GMOLE/DEG.K

      2.5000+01              4.6127+04              4.9555+01              -2.2979+01
      5.0000+01              5.9565+04              9.3543+01              -1.9839+01
      1.0000+02              5.9236+04              9.2597+01              -1.4455+01
      1.5000+02              5.8890+04              9.1727+01              -1.0368+01
      2.0000+02              5.8519+04              9.0899+01              -7.1634+00
      2.5000+02              5.8119+04              9.0095+01              -4.5887+00
      3.0000+02              5.7687+04              8.9306+01              -2.4785+00
      3.5000+02              5.7220+04              8.8527+01              -7.2034-01
      4.0000+02              5.6719+04              8.7752+01               7.6387-01
      4.5000+02              5.6180+04              8.6981+01               2.0312+00
      5.0000+02              5.5605+04              8.6212+01               3.1237+00
      5.5000+02              5.4991+04              8.5443+01               4.0732+00
      6.0000+02              5.4339+04              8.4675+01               4.9044+00
      6.5000+02              5.3649+04              8.3907+01               5.6365+00
      7.0000+02              5.2920+04              8.3138+01               6.2847+00
      7.5000+02              5.2152+04              8.2368+01               6.8614+00

          HR PLOT COMPLETED
          SR PLOT COMPLETED
          LOG K PLOT COMPLETED
```

CO(NO3)2 = N2O5 + COO



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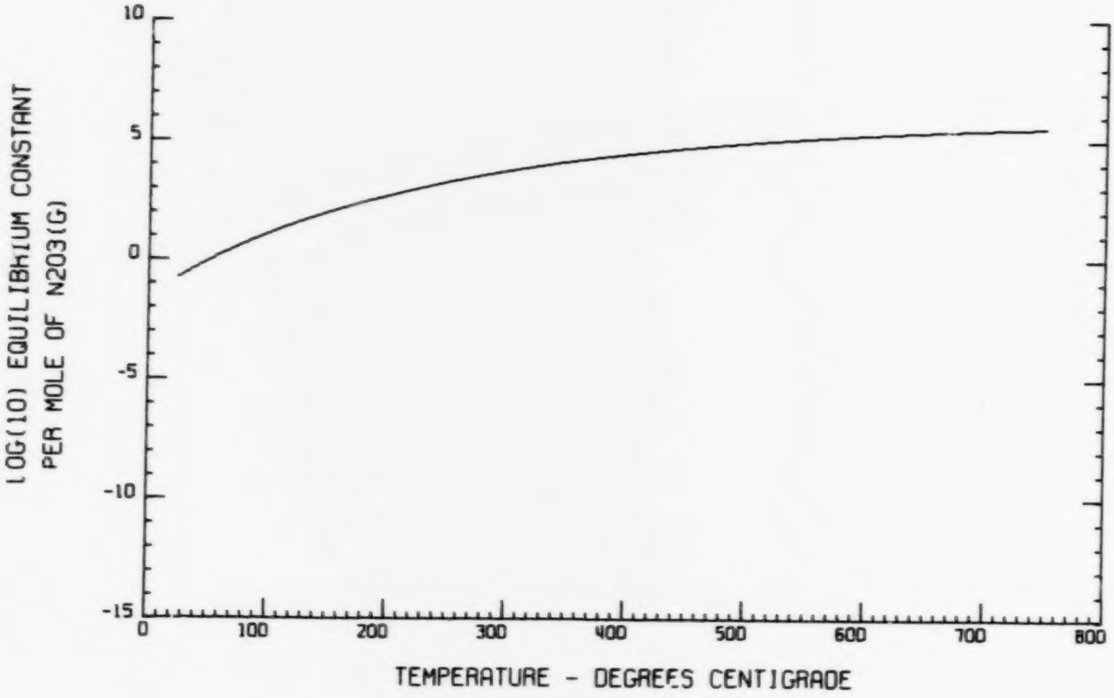
```
9 SEPT.  1971                     2CUNO2  =  N2O3 + CU2O


       TEMPERATURE              ENTHALPY              ENTROPY                 LOG  K
        DEG. C                CAL./GMOLE        CAL./GMOLE/DEG.K

       2.5000+01              1.2700+04            3.9151+01             -7.5237-01
       5.0000+01              1.2724+04            3.9230+01             -3.1640-02
       1.0000+02              1.2788+04            3.9413+01              1.1241+00
       1.5000+02              1.2830+04            3.9519+01              2.0106+00
       2.0000+02              1.2818+04            3.9494+01              2.7107+00
       2.5000+02              1.2733+04            3.9326+01              3.2750+00
       3.0000+02              1.2564+04            3.9017+01              3.7363+00
       3.5000+02              1.2300+04            3.8578+01              4.1170+00
       4.0000+02              1.1937+04            3.8018+01              4.4330+00
       4.5000+02              1.1470+04            3.7349+01              4.6961+00
       5.0000+02              1.0895+04            3.6581+01              4.9149+00
       5.5000+02              1.0211+04            3.5724+01              5.0964+00
       6.0000+02              9.4142+03            3.4786+01              5.2458+00
       6.5000+02              8.5047+03            3.3773+01              5.3675+00
       7.0000+02              7.4809+03            3.2694+01              5.4649+00
       7.5000+02              6.3417+03            3.1553+01              5.5410+00

            HR PLOT COMPLETED
            SR PLOT COMPLETED
            LOG K PLOT COMPLETED
```

2CUNO2 = N2O3 + CU2O



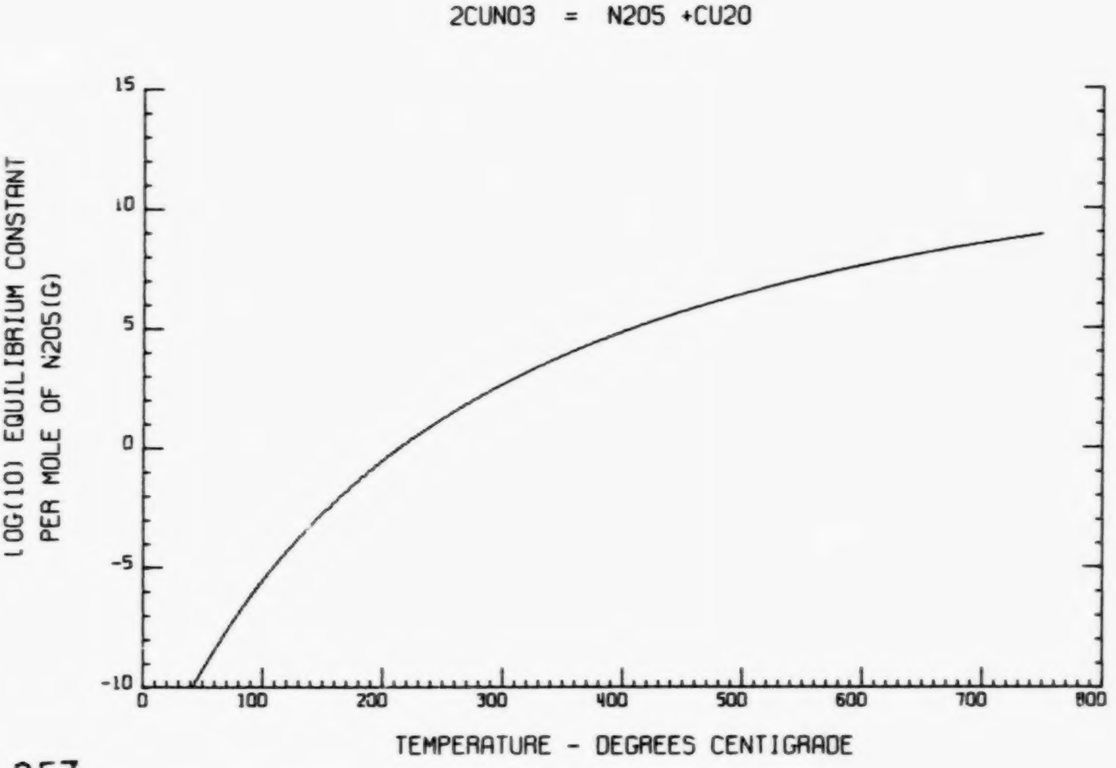
09 SEP 71

```
9 SEPT.  1971                        2CUNO3  =  N2O5 +CU2O

          TEMPERATURE              ENTHALPY              ENTROPY                LOG  K
           DEG. C                 CAL./GMOLE          CAL./GMOLE/DEG.K

          2.5000+01               2.7600+04              4.0761+01              -1.1322+01
          5.0000+01               4.1038+04              8.4749+01              -9.2314+00
          1.0000+02               4.0709+04              8.3803+01              -5.5269+00
          1.5000+02               4.0363+04              8.2932+01              -2.7212+00
          2.0000+02               3.9992+04              8.2104+01              -5.2809-01
          2.5000+02               3.9591+04              8.1300+01               1.2288+00
          3.0000+02               3.9159+04              8.0511+01               2.6640+00
          3.5000+02               3.8692+04              7.9730+01               3.8551+00
          4.0000+02               3.8190+04              7.8956+01               4.8567+00
          4.5000+02               3.7651+04              7.8184+01               5.7081+00
          5.0000+02               3.7075+04              7.7414+01               6.4385+00
          5.5000+02               3.6461+04              7.6645+01               7.0699+00
          6.0000+02               3.5809+04              7.5876+01               7.6194+00
          6.5000+02               3.5118+04              7.5107+01               8.1003+00
          7.0000+02               3.4389+04              7.4337+01               8.5231+00
          7.5000+02               3.3620+04              7.3567+01               8.8964+00

               HR PLOT COMPLETED
               SR PLOT COMPLETED
               LOG K PLOT COMPLETED
```



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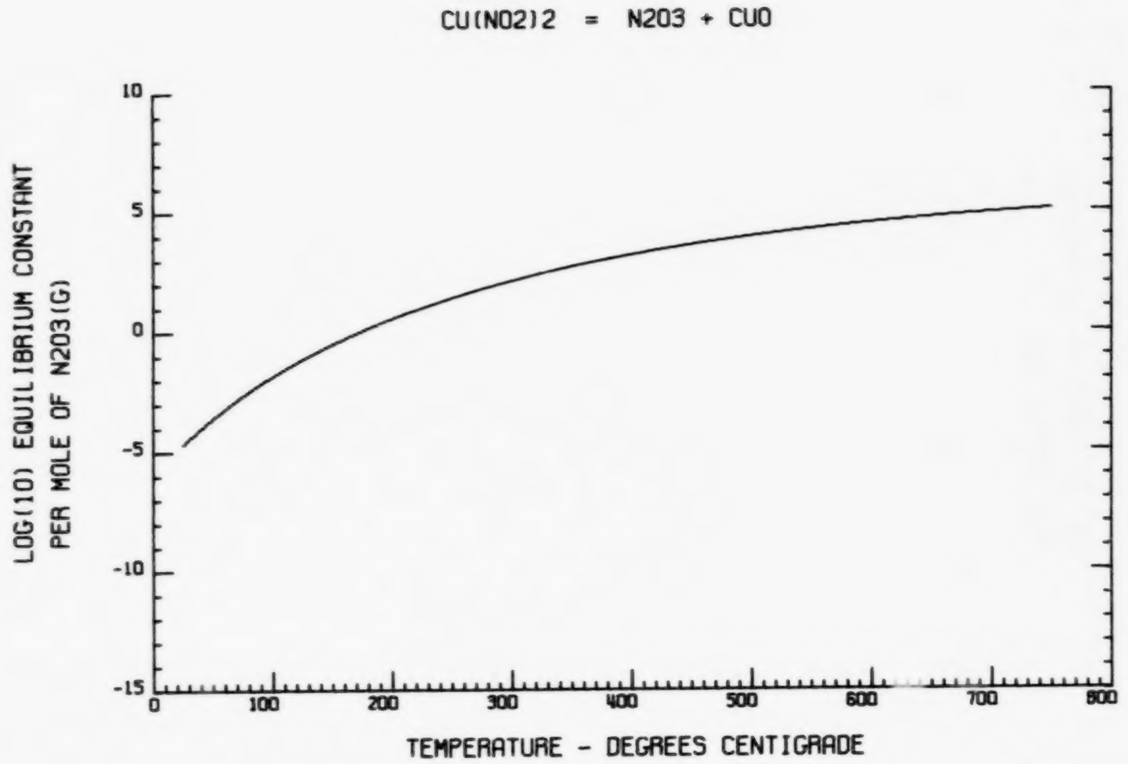
```
9 SEPT.  1971                    CU(NC2)2  =  N203 + CUO


      TEMPERATURE          ENTHALPY              ENTROPY               LOG  K
       DEG. C            CAL./GMOLE        CAL./GMOLE/DEG.K

      2.5000+01           1.9250+04            4.3300+01            -4.6467+00
      5.0000+01           1.9275+04            4.3379+01            -3.5546+00
      1.0000+02           1.9338+04            4.3562+01            -1.8053+00
      1.5000+02           1.9380+04            4.3668+01            -4.6554-01
      2.0000+02           1.9368+04            4.3643+01             5.9208-01
      2.5000+02           1.9284+04            4.3475+01             1.4455+00
      3.0000+02           1.9114+04            4.3167+01             2.1455+00
      3.5000+02           1.8851+04            4.2727+01             2.7266+00
      4.0000+02           1.8488+04            4.2168+01             3.2133+00
      4.5000+02           1.8021+04            4.1499+01             3.6233+00
      5.0000+02           1.7446+04            4.0731+01             3.9702+00
      5.5000+02           1.6761+04            3.9874+01             4.2641+00
      6.0000+02           1.5965+04            3.8936+01             4.5132+00
      6.5000+02           1.5056+04            3.7924+01             4.7237+00
      7.0000+02           1.4032+04            3.6844+01             4.9008+00
      7.5000+02           1.2893+04            3.5703+01             5.0487+00

           HR PLOT COMPLETED
           SR PLOT COMPLETED
           LOG K PLOT COMPLETED
```



09 SEP 71

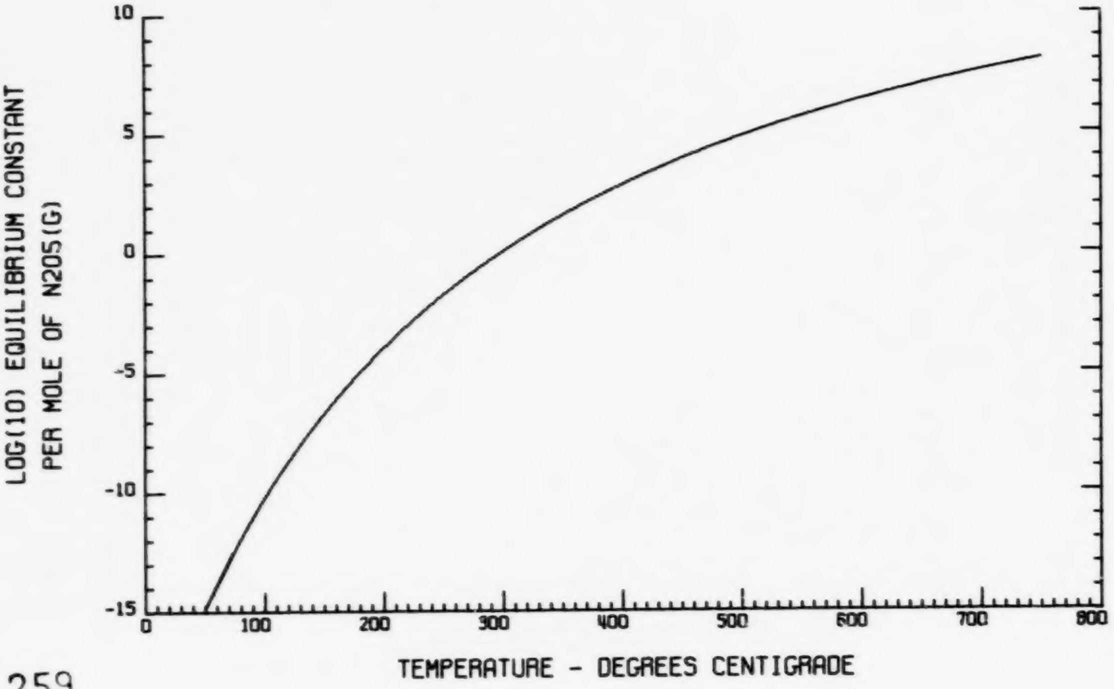
```
9 SEPT.  1971                    CU(NO3)2  =  N2O5 + CUO

    TEMPERATURE             ENTHALPY              ENTROPY                  LOG  K
     DEG. C               CAL./GMOLE         CAL./GMOLE/DEG.K

    2.5000+01             3.7850+04             4.6890+01              -1.7495+01
    5.0000+01             5.1289+04             9.0878+01              -1.4824+01
    1.0000+02             5.0960+04             8.9933+01              -1.0190+01
    1.5000+02             5.0613+04             8.9062+01              -6.6755+00
    2.0000+02             5.0242+04             8.8234+01              -3.9229+00
    2.5000+02             4.9842+04             8.7431+01              -1.7135+00
    3.0000+02             4.9410+04             8.6642+01               9.5252-02
    3.5000+02             4.8944+04             8.5863+01               1.6000+00
    4.0000+02             4.8442+04             8.5088+01               2.8686+00
    4.5000+02             4.7904+04             8.4317+01               3.9501+00
    5.0000+02             4.7328+04             8.3548+01               4.8809+00
    5.5000+02             4.6715+04             8.2779+01               5.6884+00
    6.0000+02             4.6063+04             8.2011+01               6.3938+00
    6.5000+02             4.5373+04             8.1242+01               7.0136+00
    7.0000+02             4.4643+04             8.0473+01               7.5612+00
    7.5000+02             4.3875+04             7.9704+01               8.0470+00

         HR PLOT COMPLETED
         SR PLOT COMPLETED
         LOG K PLOT COMPLETED
```

CU(NO3)2 = N2O5 + CUO



09 SEP 71

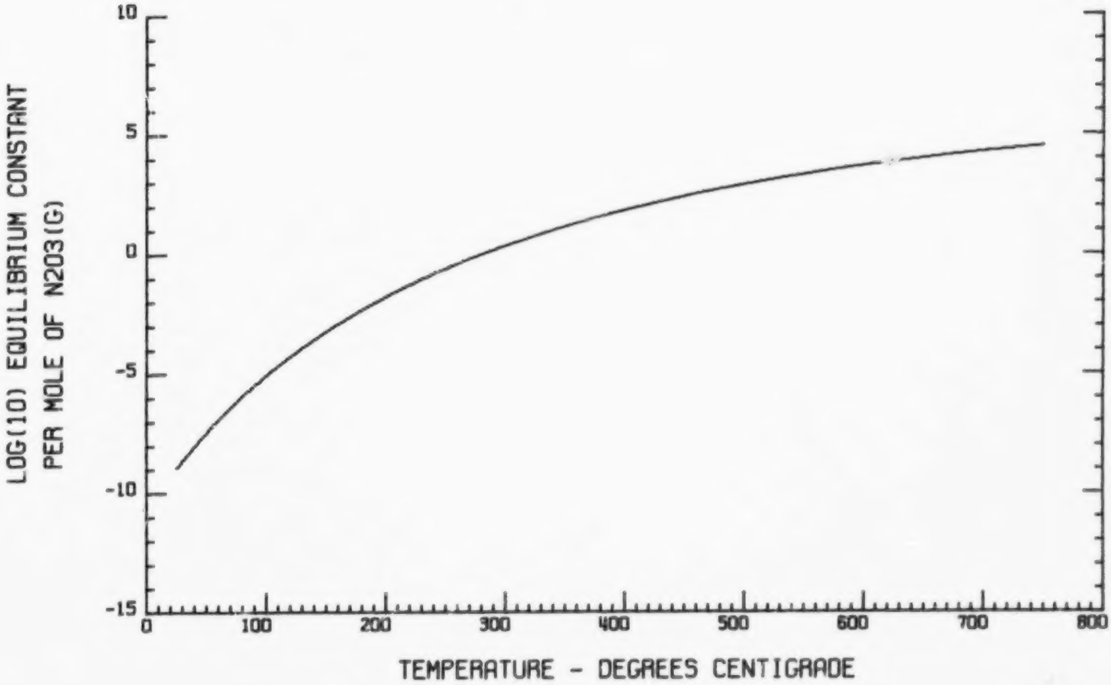
```
9 SEPT.  1971                          FE(NO2)2  =  N2O3 + FEO


      TEMPERATURE                 ENTHALPY                 ENTROPY                    LOG  K
       DEG. C                    CAL./GMOLE           CAL./GMOLE/DEG.K

       2.5000+01                 2.6398+04                4.7701+01                -8.9239+00
       5.0000+01                 2.6422+04                4.7779+01                -7.4265+00
       1.0000+02                 2.6486+04                4.7962+01                -5.0296+00
       1.5000+02                 2.6527+04                4.8068+01                -3.1952+00
       2.0000+02                 2.6516+04                4.8043+01                -1.7475+00
       2.5000+02                 2.6431+04                4.7875+01                -5.7854-01
       3.0000+02                 2.6262+04                4.7567+01                 3.8192-01
       3.5000+02                 2.5998+04                4.7127+01                 1.1817+00
       4.0000+02                 2.5635+04                4.6568+01                 1.8545+00
       4.5000+02                 2.5168+04                4.5899+01                 2.4250+00
       5.0000+02                 2.4593+04                4.5131+01                 2.9115+00
       5.5000+02                 2.3909+04                4.4274+01                 3.3282+00
       6.0000+02                 2.3112+04                4.3336+01                 3.6859+00
       6.5000+02                 2.2203+04                4.2324+01                 3.9935+00
       7.0000+02                 2.1179+04                4.1244+01                 4.2573+00
       7.5000+02                 2.0040+04                4.0103+01                 4.4837+00

            HR PLOT COMPLETED
            SR PLOT COMPLETED
            LOG K PLOT COMPLETED
```

FE(NO2)2 = N2O3 + FEO



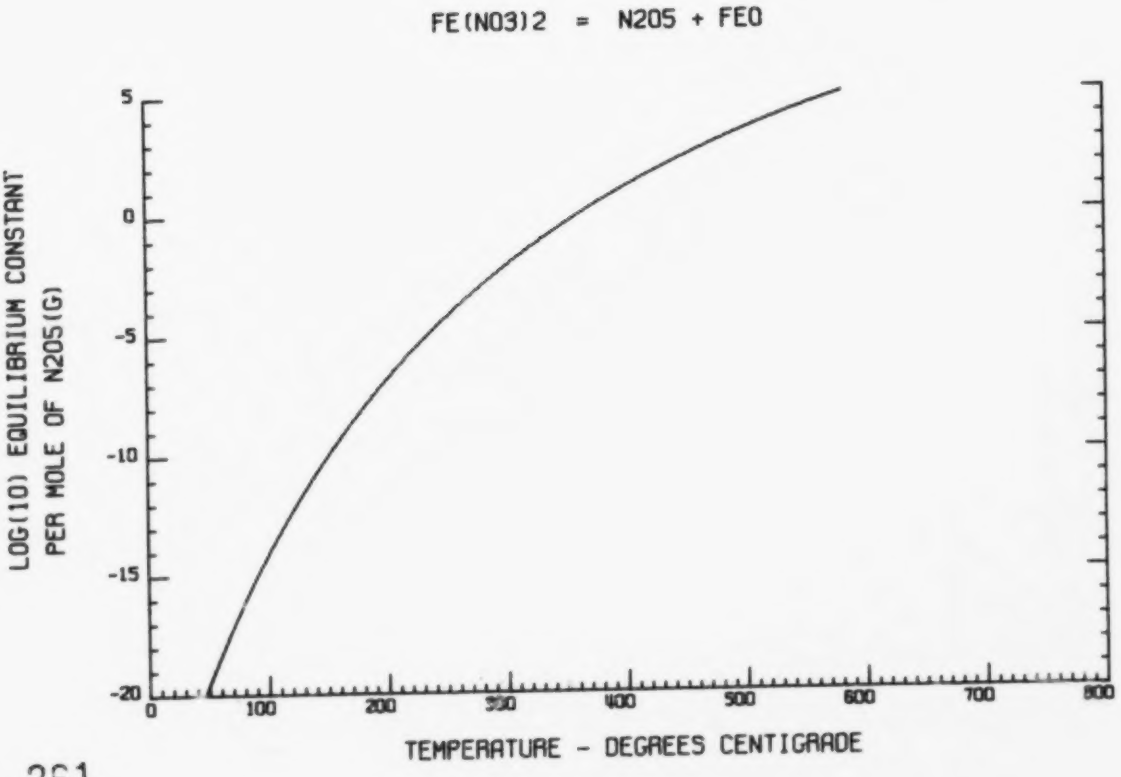
09 SEP 71

```
9 SEPT.  1971                          FE(NO3)2  =  N205 + FEO

      TEMPERATURE             ENTHALPY              ENTROPY                LOG  K
       DEG. C                CAL./GMOLE        CAL./GMOLE/DEG.K

      2.5000+01              4.6168+04             5.1291+01             -2.2630+01
      5.0000+01              5.9606+04             9.5279+01             -1.9487+01
      1.0000+02              5.9277+04             9.4333+01             -1.4100+01
      1.5000+02              5.8931+04             9.3465+01             -1.0009+01
      2.0000+02              5.8560+04             9.2635+01             -6.8028+00
      2.5000+02              5.8160+04             9.1832+01             -4.2265+00
      3.0000+02              5.7728+04             9.1043+01             -2.1144+00
      3.5000+02              5.7261+04             9.0263+01             -3.5519-01
      4.0000+02              5.6759+04             8.9489+01              1.1301+00
      4.5000+02              5.6221+04             8.8718+01              2.3983+00
      5.0000+02              5.5645+04             8.7949+01              3.4916+00
      5.5000+02              5.5032+04             8.7180+01              4.4419+00
      6.0000+02              5.4380+04             8.6412+01              5.2737+00
      6.5000+02              5.3690+04             8.5643+01              6.0064+00
      7.0000+02              5.2961+04             8.4874+01              6.6551+00
      7.5000+02              5.2193+04             8.4105+01              7.2322+00

         HR PLOT COMPLETED
         SR PLOT COMPLETED
         LOG K PLOT COMPLETED
```



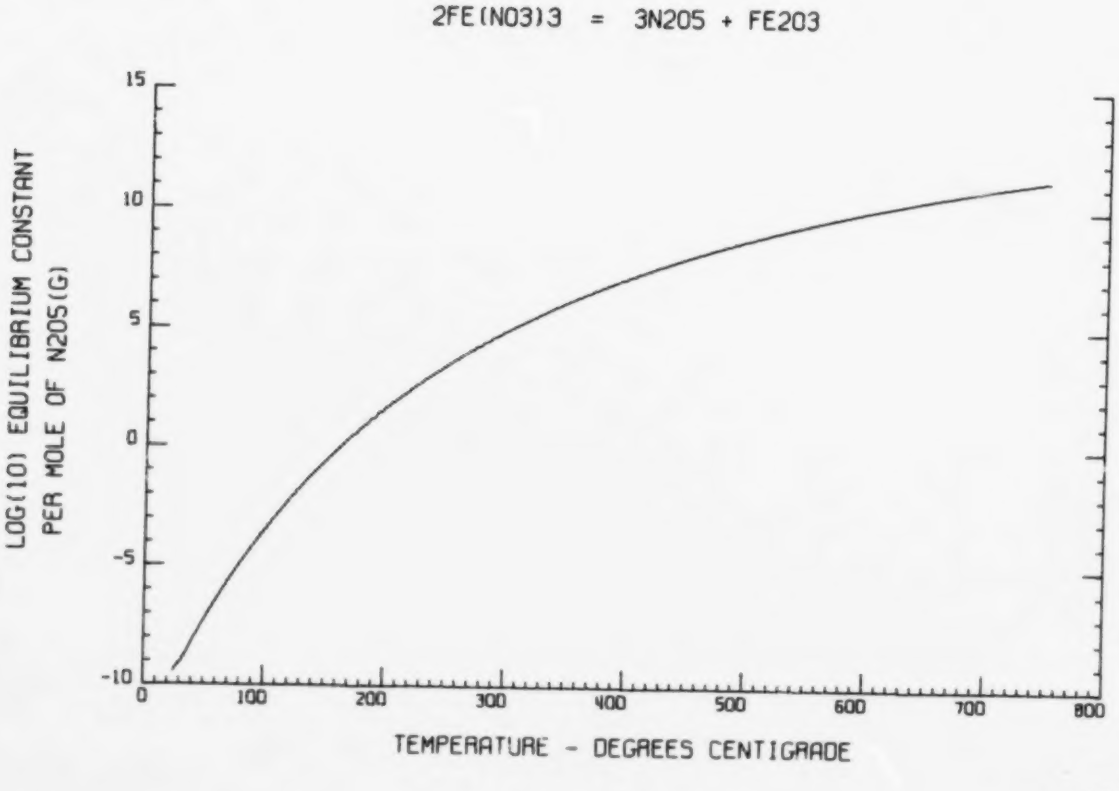
09 SEP 71

```
9 SEPT.  1971                       2FE(NO3)3  =  3N205 + FE203

      TEMPERATURE           ENTHALPY              ENTROPY                 LOG  K
       DEG. C              CAL./GMOLE        CAL./GMOLE/DEG.K

      2.5000+01            2.8565+04            5.2827+01             -9.3927+00
      5.0000+01            4.2028+04            9.6892+01             -7.2469+00
      1.0000+02            4.1711+04            9.5981+01             -3.4520+00
      1.5000+02            4.1348+04            9.5071+01             -5.7740-01
      2.0000+02            4.0948+04            9.4179+01              1.6688+00
      2.5000+02            4.0517+04            9.3312+01              3.4673+00
      3.0000+02            4.0056+04            9.2471+01              4.9357+00
      3.5000+02            3.9568+04            9.1656+01              6.1539+00
      4.0000+02            3.9056+04            9.0865+01              7.1782+00
      4.5000+02            3.8520+04            9.0097+01              8.0490+00
      5.0000+02            3.7960+04            8.9349+01              8.7965+00
      5.5000+02            3.7378+04            8.8619+01              9.4434+00
      6.0000+02            3.6774+04            8.7907+01              1.0007+01
      6.5000+02            3.6148+04            8.7210+01              1.0502+01
      7.0000+02            3.5516+04            8.6544+01              1.0938+01
      7.5000+02            3.4753+04            8.5779+01              1.1323+01

          HR PLOT COMPLETED
          SR PLOT COMPLETED
          LOG K PLOT COMPLETED
```



09 SEP 71

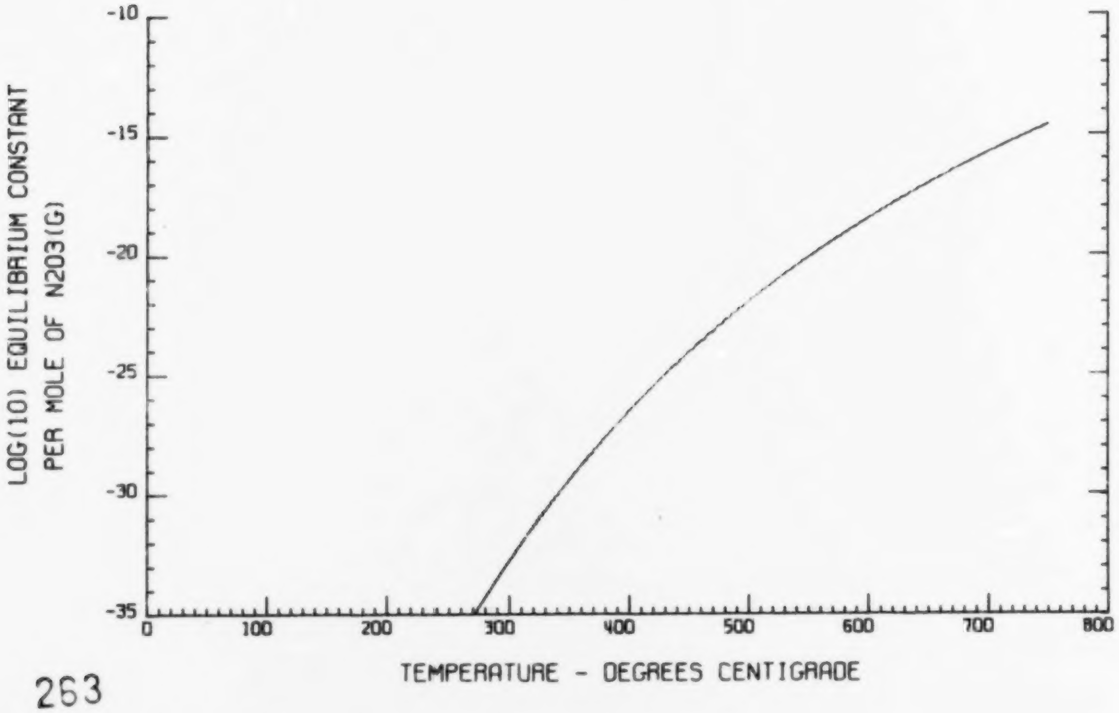
```
9 SEPT.  1971                        2KNO2  =  N2O3 + K2O

  TEMPERATURE           ENTHALPY              ENTROPY             LOG  K
   DEG. C              CAL./GMOLE        CAL./GMOLE/DEG.K

  2.5000+01            1.1040+05            4.3314+01          -7.1451+01
  5.0000+01            1.1002+05            4.2150+01          -6.5193+01
  1.0000+02            1.1009+05            4.2333+01          -5.5221+01
  1.5000+02            1.1013+05            4.2439+01          -4.7601+01
  2.0000+02            1.1012+05            4.2414+01          -4.1591+01
  2.5000+02            1.1003+05            4.2246+01          -3.6732+01
  3.0000+02            1.0986+05            4.1938+01          -3.2725+01
  3.5000+02            1.0960+05            4.1499+01          -2.9367+01
  4.0000+02            1.0924+05            4.0939+01          -2.6517+01
  4.5000+02            1.0877+05            4.0271+01          -2.4070+01
  5.0000+02            1.0820+05            3.9503+01          -2.1949+01
  5.5000+02            1.0751+05            3.8646+01          -2.0097+01
  6.0000+02            1.0672+05            3.7708+01          -1.8469+01
  6.5000+02            1.0581+05            3.6696+01          -1.7028+01
  7.0000+02            1.0478+05            3.5616+01          -1.5747+01
  7.5000+02            1.0364+05            3.4475+01          -1.4603+01

       HR PLOT COMPLETED
       SR PLOT COMPLETED
       LOG K PLOT COMPLETED
```

2KNO2 = N2O3 + K2O



09 SEP 71

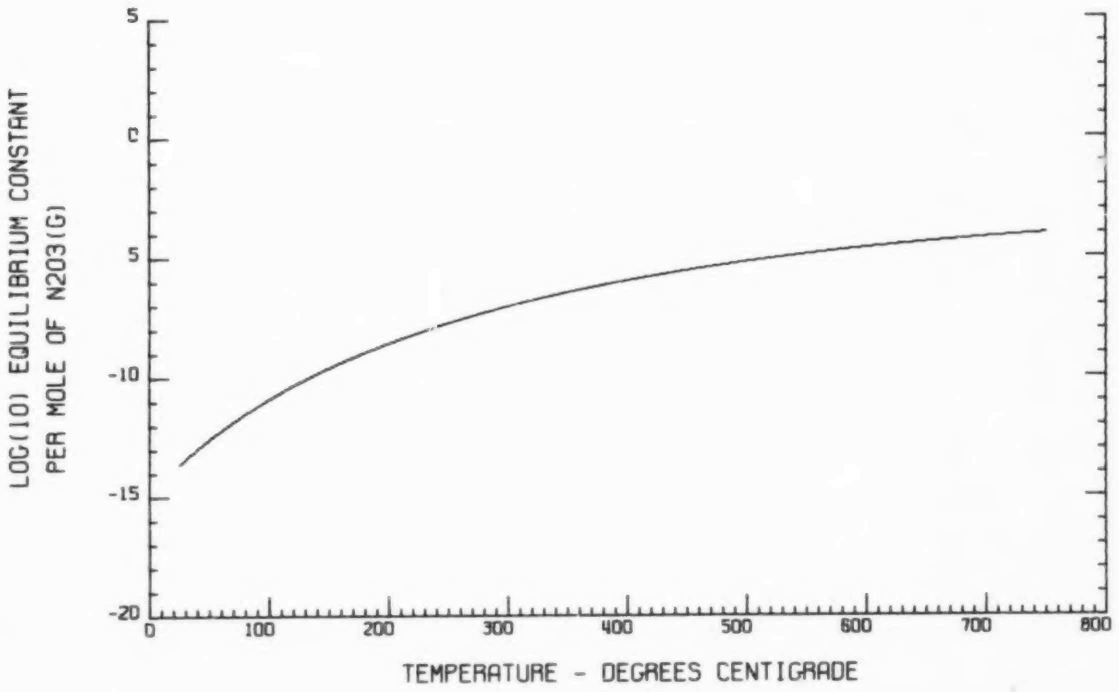
```
8  OCT.  1971                2KNO2 + CO2  I  N2O3(G) + K2CO3


      TEMPERATURE             ENTHALPY               ENTROPY                 LOG  K
        DEG. C               CAL./GMOLE         CAL./GMOLE/DEG.K

      2.5000+01              1.8901+04             1.0646+00             -1.3621+01
      5.0000+01              1.8521+04            -1.2233-01             -1.2552+01
      1.0000+02              1.8628+04             1.8405-01             -1.0869+01
      1.5000+02              1.8767+04             5.3254-01             -9.5757+00
      2.0000+02              1.8888+04             8.0432-01             -8.5582+00
      2.5000+02              1.8963+04             9.5468-01             -7.7126+00
      3.0000+02              1.8971+04             9.7069-01             -7.0212+00
      3.5000+02              1.8900+04             8.5339-01             -6.4417+00
      4.0000+02              1.8742+04             6.0977-01             -5.9512+00
      4.5000+02              1.8489+04             2.4905-01             -5.5331+00
      5.0000+02              1.8139+04            -2.1899-01             -5.1749+00
      5.5000+02              1.7687+04            -7.8489-01             -4.8672+00
      6.0000+02              1.7131+04            -1.4398+00             -4.6023+00
      6.5000+02              1.6470+04            -2.1757+00             -4.3745+00
      7.0000+02              1.5702+04            -2.9852+00             -4.1785+00
      7.5000+02              1.4827+04            -3.8618+00             -4.0108+00

          HR PLOT COMPLETED
          SH PLOT COMPLETED
          LOG K PLOT COMPLETED
```

2KNO2 + CO2 → N2O3(G) + K2CO3

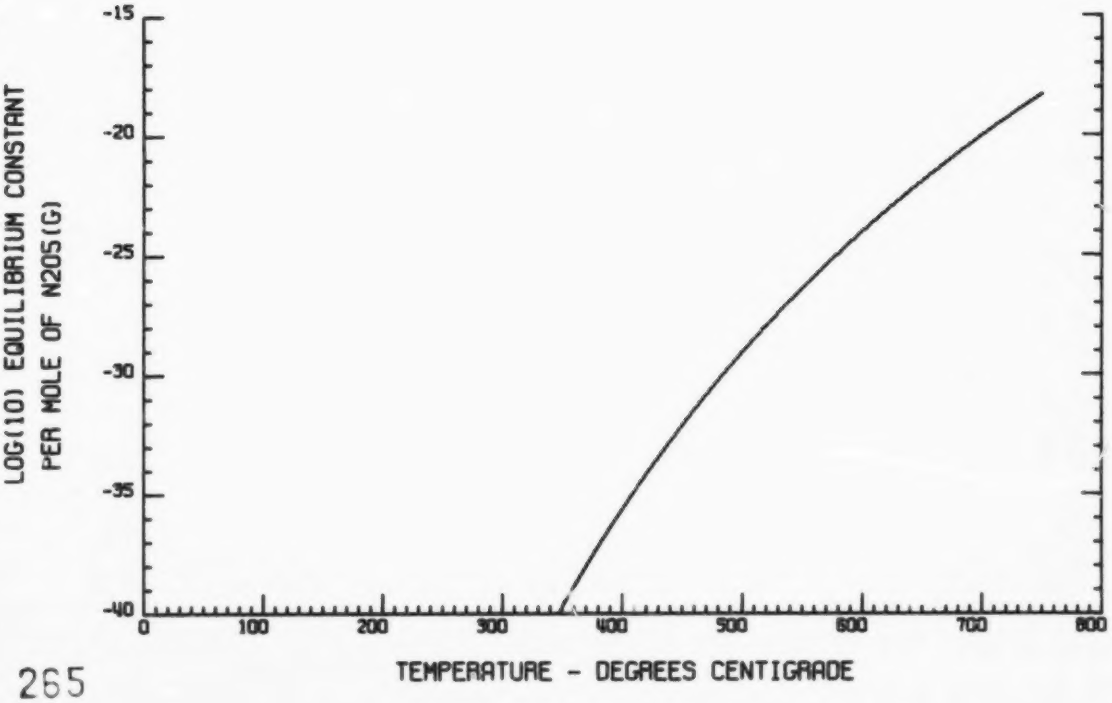


19 AUG. 1971

2KN03 = N205 +K20

TEMPERATURE DEG. C	ENTHALPY CAL./GMOLE	ENTROPY CAL./GMOLE/DEG.K	LOG K
2.5000+01	1.5174+05	4.2764+01	-1.0187+02
5.0000+01	1.6519+05	8.6807+01	-9.2745+01
1.0000+02	1.6496+05	8.6137+01	-7.7784+01
1.5000+02	1.6219+05	7.9242+01	-6.6447+01
2.0000+02	1.6180+05	7.8366+01	-5.7606+01
2.5000+02	1.6150+05	7.7765+01	-5.0471+01
3.0000+02	1.6126+05	7.7352+01	-4.4589+01
3.5000+02	1.5649+05	6.9470+01	-3.9700+01
4.0000+02	1.5632+05	6.9134+01	-3.5626+01
4.5000+02	1.5619+05	6.9007+01	-3.2119+01
5.0000+02	1.5610+05	6.8891+01	-2.9067+01
5.5000+02	1.5605+05	6.8832+01	-2.6388+01
6.0000+02	1.5604+05	6.8821+01	-2.4015+01
6.5000+02	1.5607+05	6.8851+01	-2.1900+01
7.0000+02	1.5613+05	6.8915+01	-2.0001+01
7.5000+02	1.5623+05	6.9009+01	-1.8287+01

2KN03 = N205 +K20



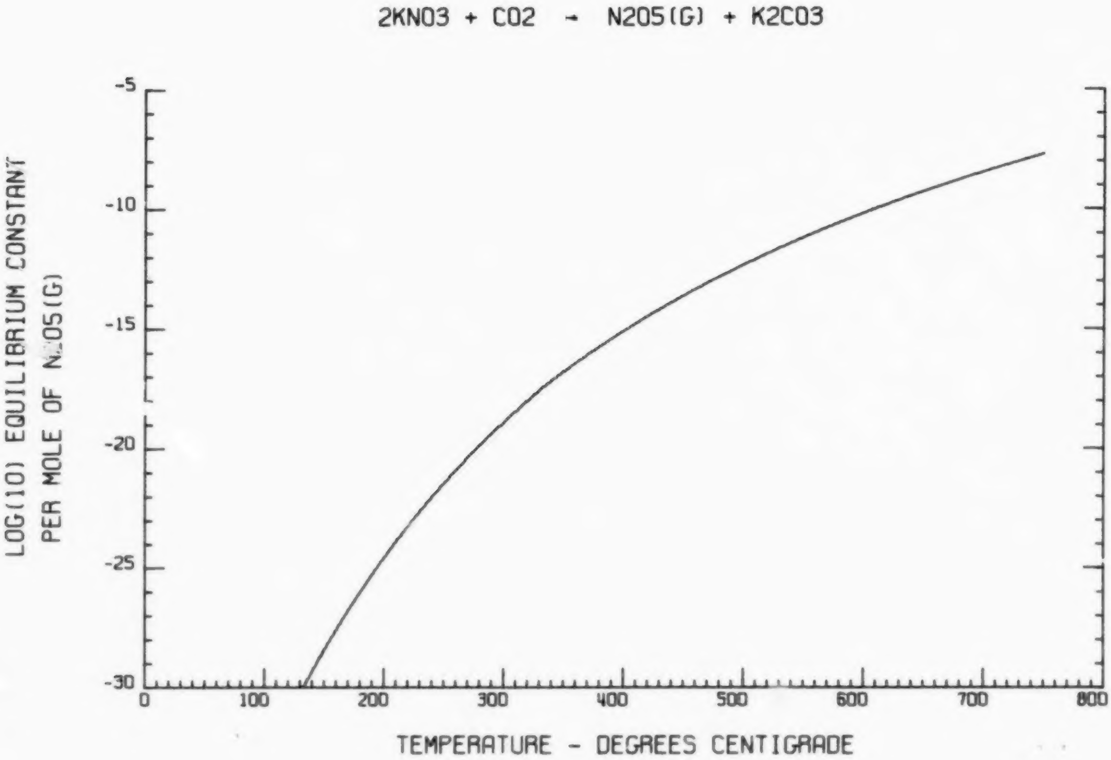
10 AUG 71

```
8  OCT.  1971                    2KNO3 + CO2  I  N2O5(G) + K2CO3

          TEMPERATURE               ENTHALPY                 ENTROPY                      LOG  K
           DEG. C                  CAL./GMOLE           CAL./GMOLE/DEG.K

          2.5000+01                6.0241+04                5.1464-01                 -4.4042+01
          5.0000+01                7.3690+04                4.4535+01                 -4.0101+01
          1.0000+02                7.3502+04                4.3988+01                 -3.5455+01
          1.5000+02                7.0832+04                3.7336+01                 -2.8422+01
          2.0000+02                7.0574+04                3.6758+01                 -2.4563+01
          2.5000+02                7.0433+04                3.6473+01                 -2.1451+01
          3.0000+02                7.0385+04                3.6384+01                 -1.8886+01
          3.5000+02                6.5793+04                2.8825+01                 -1.6774+01
          4.0000+02                6.5619+04                2.8864+01                 -1.5060+01
          4.5000+02                6.5904+04                2.8985+01                 -1.3582+01
          5.0000+02                6.6041+04                2.9168+01                 -1.2293+01
          5.5000+02                6.6227+04                2.9401+01                 -1.1157+01
          6.0000+02                6.6458+04                2.9674+01                 -1.0149+01
          6.5000+02                6.6733+04                2.9979+01                 -9.2460+00
          7.0000+02                6.7050+04                3.0313+01                 -8.4325+00
          7.5000+02                6.7407+04                3.0671+01                 -7.6948+00

                HR PLOT COMPLETED
                SR PLOT COMPLETED
                LOG K PLOT COMPLETED
```



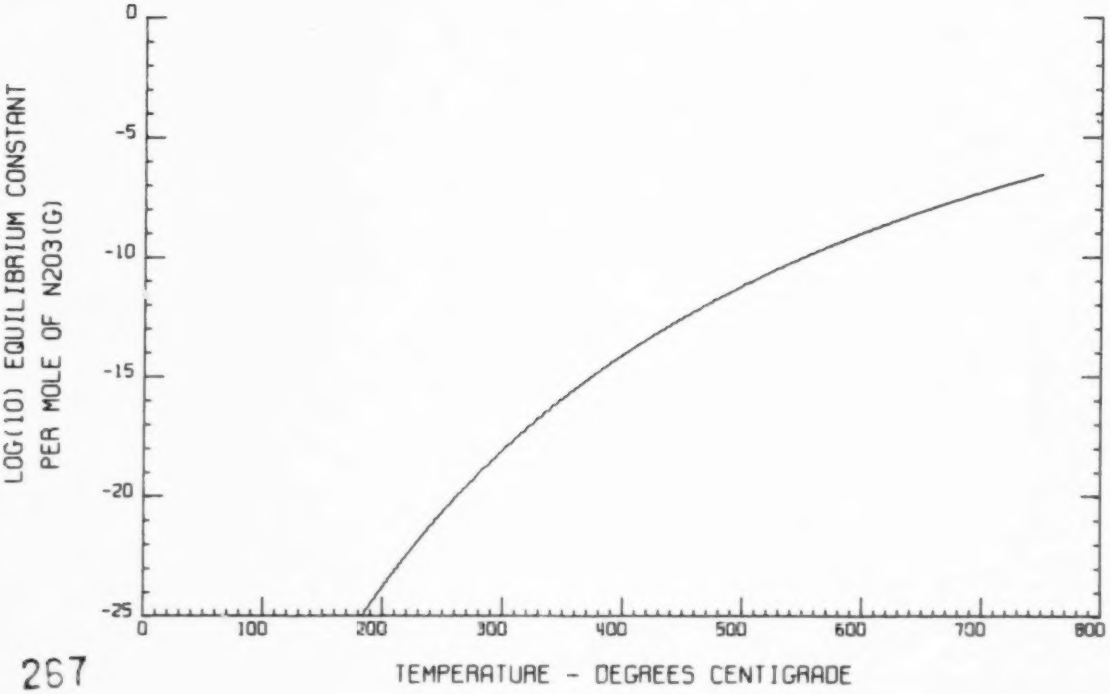
```
9 SEPT.  1971                          2LINO2  =  N203 + LI20


     TEMPERATURE              ENTHALPY                  ENTROPY                    LOG  K
      DEG. C                CAL./GMOLE             CAL./GMOLE/DEG.K

     2.5000+01              7.0496+04                 4.0282+01                -4.2868+01
     5.0000+01              7.0521+04                 4.0361+01                -3.8870+01
     1.0000+02              7.0584+04                 4.0543+01                -3.2477+01
     1.5000+02              7.0626+04                 4.0649+01                -2.7591+01
     2.0000+02              7.0614+04                 4.0624+01                -2.3737+01
     2.5000+02              7.0530+04                 4.0456+01                -2.0621+01
     3.0000+02              7.0360+04                 4.0148+01                -1.8054+01
     3.5000+02              7.0097+04                 3.9708+01                -1.5905+01
     4.0000+02              6.9734+04                 3.9148+01                -1.4083+01
     4.5000+02              6.9266+04                 3.8479+01                -1.2523+01
     5.0000+02              6.8691+04                 3.7712+01                -1.1175+01
     5.5000+02              6.8007+04                 3.6854+01                -1.0001+01
     6.0000+02              6.7211+04                 3.5916+01                -8.9728+00
     6.5000+02              6.6301+04                 3.4903+01                -8.0676+00
     7.0000+02              6.5277+04                 3.3824+01                -7.2672+00
     7.5000+02              6.4138+04                 3.2683+01                -6.5569+00

          HR PLOT COMPLETED
          SR PLOT COMPLETED
          LOG K PLOT COMPLETED
```

2LINO2 = N203 + LI20



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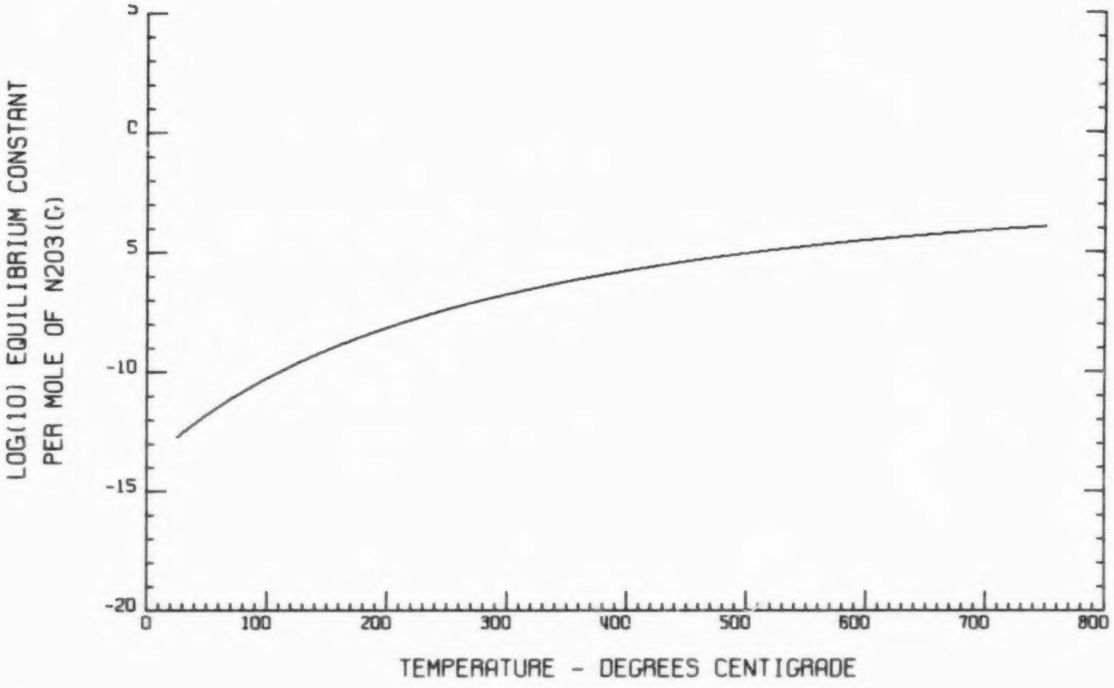
```
8  OCT.  1971                    2LINO2 + CO2  I  N2O3(G) + LI2CO3

      TEMPERATURE              ENTHALPY              ENTROPY                  LOG  K
       DEG. C                CAL./GMOLE         CAL./GMOLE/DEG.K

      2.5000+01              1.6746+04            -2.0270+00              -1.2717+01
      5.0000+01              1.6794+04            -1.8735+00              -1.1766+01
      1.0000+02              1.6907+04            -1.5485+00              -1.0240+01
      1.5000+02              1.7028+04            -1.2434+00              -9.0659+00
      2.0000+02              1.7146+04            -9.7922-01              -8.1355+00
      2.5000+02              1.7255+04            -7.6146-01              -7.3742+00
      3.0000+02              1.7349+04            -5.8926-01              -6.7437+00
      3.5000+02              1.7426+04            -4.5944-01              -6.2118+00
      4.0000+02              1.7486+04            -3.6794-01              -5.7571+00
      4.5000+02              1.7259+04            -6.9036-01              -5.3664+00
      5.0000+02              1.6933+04            -1.1248+00              -5.0322+00
      5.5000+02              1.6575+04            -1.5744+00              -4.7444+00
      6.0000+02              1.6181+04            -2.0382+00              -4.4953+00
      6.5000+02              1.5753+04            -2.5153+00              -4.2788+00
      7.0000+02              1.5289+04            -3.0046+00              -4.0899+00
      7.5000+02              1.4789+04            -3.5049+00              -3.9248+00

          HR PLOT COMPLETED
          SR PLOT COMPLETED
          LOG K PLOT COMPLETED
```

2LINO2 + CO2 - N2O3(G) + LI2CO3



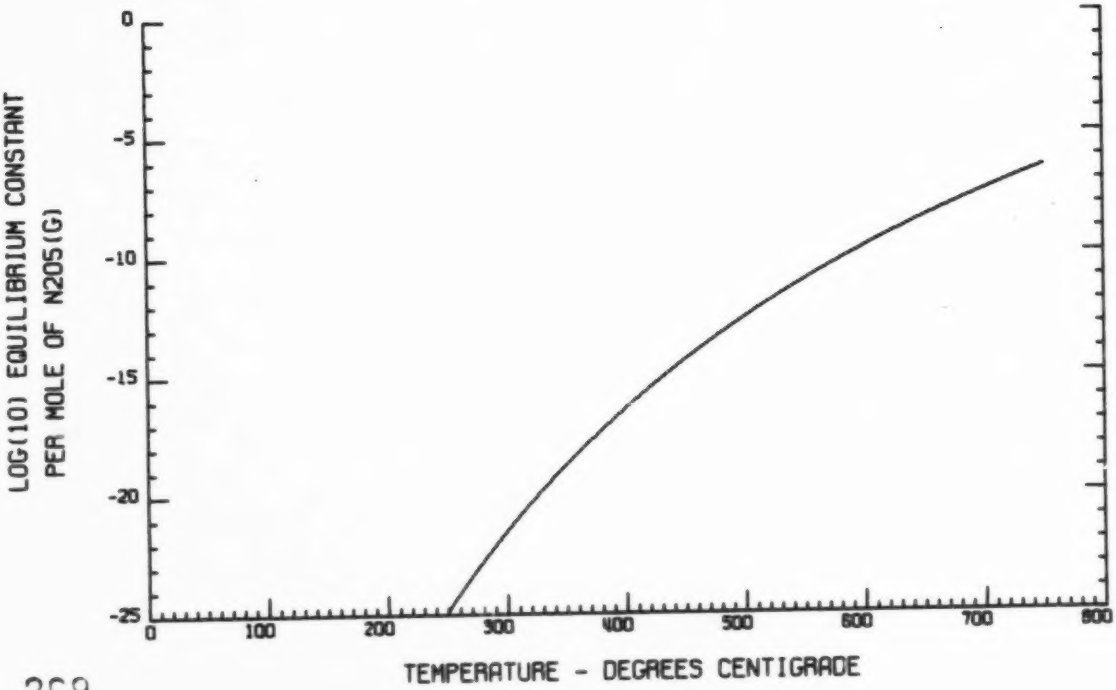
08 OCT 71

19 ALG. 1971

2LINO3 = N205 + LI2O

TEMPERATURE DEG. C	ENTHALPY CAL./GMOLE	ENTROPY CAL./GMOLE/DEG.K	LOG K
2.5000+01	9.0596+04	4.1892+01	-5.7248+01
5.0000+01	1.0397+05	8.5655+01	-5.1586+01
1.0000+02	1.0361+05	8.4634+01	-4.2184+01
1.5000+02	1.0333+05	8.3934+01	-3.5023+01
2.0000+02	1.0306+05	8.3365+01	-2.9391+01
2.5000+02	1.0282+05	8.2636+01	-2.4846+01
3.0000+02	9.0445+04	5.9347+01	-2.1516+01
3.5000+02	9.0215+04	5.6960+01	-1.8753+01
4.0000+02	9.0036+04	5.6685+01	-1.6405+01
4.5000+02	8.9902+04	5.6491+01	-1.4366+01
5.0000+02	8.9807+04	5.6364+01	-1.2630+01
5.5000+02	8.9748+04	5.6290+01	-1.1088+01
6.0000+02	8.9721+04	5.6256+01	-9.7242+00
6.5000+02	8.9724+04	5.6261+01	-8.5080+00
7.0000+02	8.9754+04	5.6293+01	-7.4165+00
7.5000+02	8.9811+04	5.6350+01	-6.4313+00

2LINO3 = N205 + LI20



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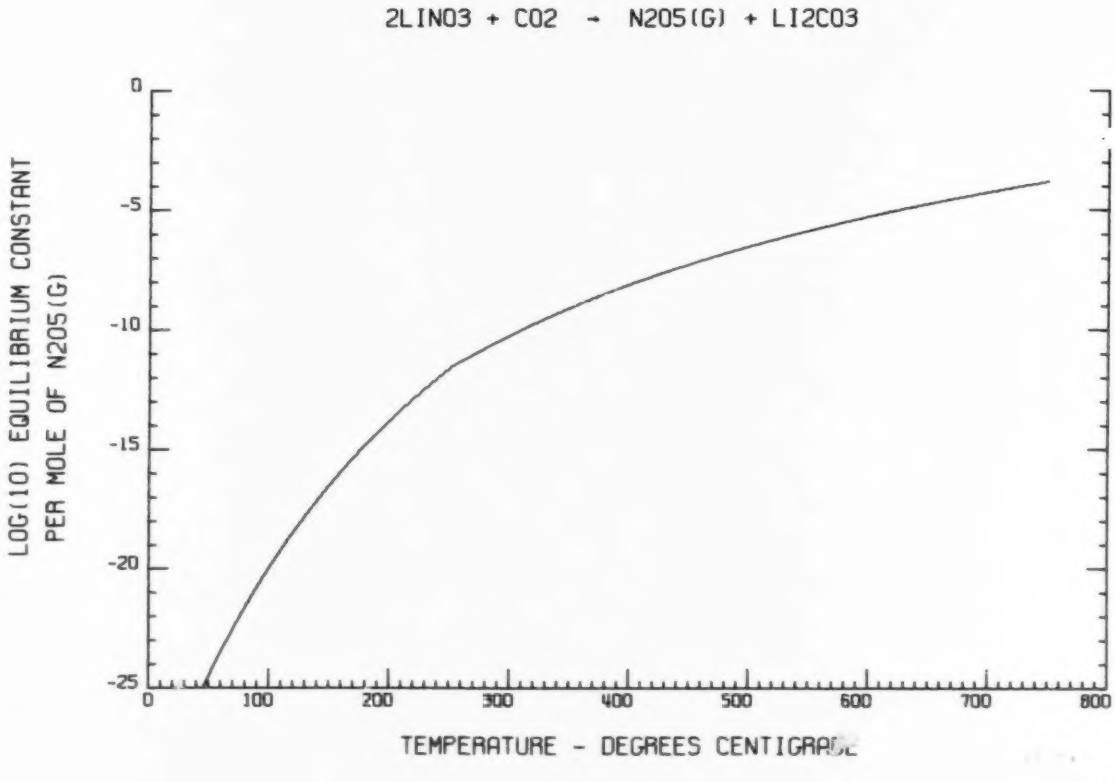
10 AUG 71

```
8  OCT.  1971                    2LINO3 + CO2  I  N2O5(6) + LI2CO3

       TEMPERATURE              ENTHALPY              ENTROPY                LOG  K
        DEG. C                 CAL./GMOLE         CAL./GMOLE/DEG.K

       2.5000+01               3.6846+04            -4.1703-01            -2.7098+01
       5.0000+01               5.0238+04             4.3421+01            -2.4485+01
       1.0000+02               4.9934+04             4.2542+01            -1.9947+01
       1.5000+02               4.9736+04             4.2041+01            -1.6498+01
       2.0000+02               4.9611+04             4.1761+01            -1.3788+01
       2.5000+02               4.9540+04             4.1618+01            -1.1599+01
       3.0000+02               3.7454+04             1.8610+01            -1.0206+01
       3.5000+02               3.7544+04             1.8792+01            -9.0597+00
       4.0000+02               3.7788+04             1.9167+01            -8.0790+00
       4.5000+02               3.7694+04             1.9321+01            -7.2292+00
       5.0000+02               3.8049+04             1.9527+01            -6.4873+00
       5.5000+02               3.8516+04             1.9861+01            -5.8320+00
       6.0000+02               3.8691+04             2.0303+01            -5.2468+00
       6.5000+02               3.9175+04             2.0842+01            -4.7192+00
       7.0000+02               3.9766+04             2.1464+01            -4.2393+00
       7.5000+02               4.0463+04             2.2162+01            -3.7993+00

            HR PLOT COMPLETED
            SR PLOT COMPLETED
            LOG K PLOT COMPLETED
```



08 OCT 71

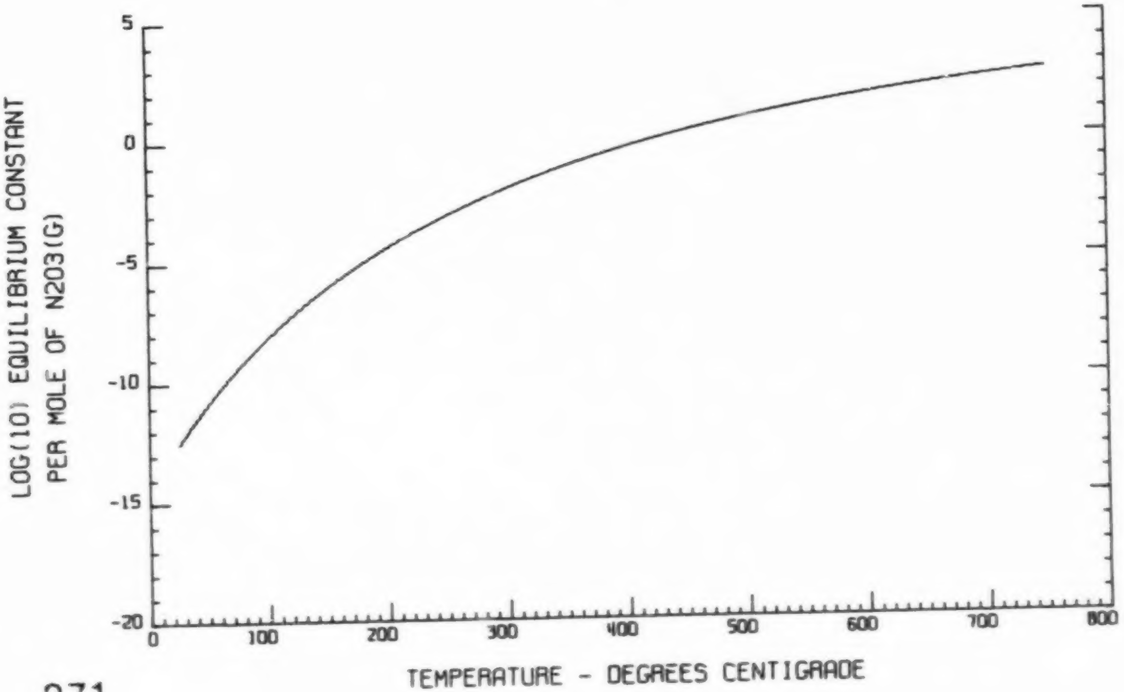
```
9 SEPT.  1971                         MG(NO2)2  =  N2O3 + MGO


   TEMPERATURE              ENTHALPY               ENTROPY              LOG  K
    DEG. C                 CAL./GMOLE        CAL./GMOLE/DEG.K

   2.5000+01               2.9803+04              4.2713+01          -1.2510+01
   5.0000+01               2.9828+04              4.2791+01          -1.0820+01
   1.0000+02               2.9691+04              4.2974+01          -8.1142+00
   1.5000+02               2.9933+04              4.3080+01          -6.0442+00
   2.0000+02               2.9921+04              4.3055+01          -4.4106+00
   2.5000+02               2.9837+04              4.2887+01          -3.0913+00
   3.0000+02               2.9667+04              4.2578+01          -2.0068+00
   3.5000+02               2.9404+04              4.2139+01          -1.1028+00
   4.0000+02               2.9041+04              4.1579+01          -3.4128-01
   4.5000+02               2.8573+04              4.0911+01           3.0565-01
   5.0000+02               2.7999+04              4.0143+01           8.5875-01
   5.5000+02               2.7314+04              3.9286+01           1.3339+00
   6.0000+02               2.6518+04              3.8347+01           1.7433+00
   6.5000+02               2.5608+04              3.7335+01           2.0969+00
   7.0000+02               2.4585+04              3.6255+01           2.4025+00
   7.5000+02               2.3446+04              3.5114+01           2.6661+00

        HR PLOT COMPLETED
        SR PLOT COMPLETED
        LOG K PLOT COMPLETED
```

MG(NO2)2 = N2O3 + MGO



09 SEP 71

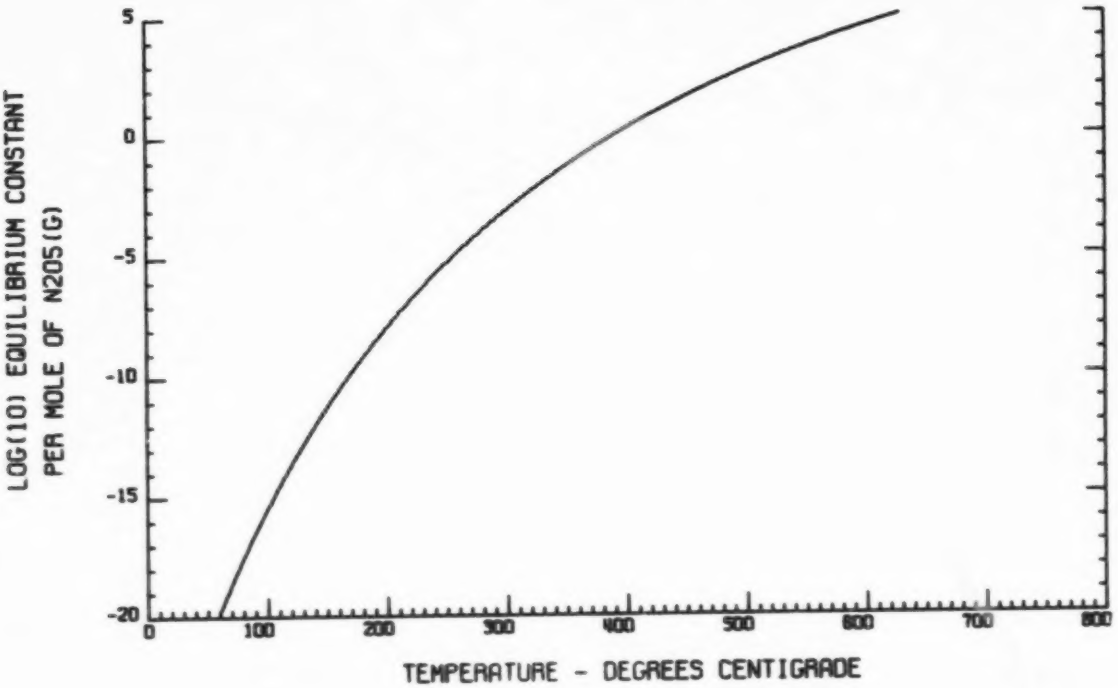
```
19 AUG. 1971                          MG(NO3)2  =  N2O5 + MGO

      TEMPERATURE          ENTHALPY             ENTROPY              LOG  K
       DEG. C             CAL./GMOLE        CAL./GMOLE/DEG.K

      2.5000+01           4.8643+04            5.0003+01           -2.4286+01
      5.0000+01           6.1521+04            9.4116+01           -2.1036+01
      1.0000+02           6.1321+04            9.3540+01           -1.5470+01
      1.5000+02           6.1113+04            9.3017+01           -1.1234+01
      2.0000+02           6.0844+04            9.2419+01           -7.9050+00
      2.5000+02           6.0484+04            9.1697+01           -5.2265+00
      3.0000+02           6.0010+04            9.0834+01           -3.0305+00
      3.5000+02           5.9410+04            8.9831+01           -1.2031+00
      4.0000+02           5.8672+04            8.8694+01            3.3534-01
      4.5000+02           5.7791+04            8.7432+01            1.6429+00
      5.0000+02           5.6759+04            8.6054+01            2.7627+00
      5.5000+02           5.5575+04            8.4570+01            3.7275+00
      6.0000+02           5.4235+04            8.2989+01            4.5626+00
      6.5000+02           5.2732+04            8.1318+01            5.2680+00
      7.0000+02           5.1071+04            7.9566+01            5.9196+00
      7.5000+02           4.9246+04            7.7739+01            6.4703+00

          HR PLOT COMPLETED
          SR PLOT COMPLETED
          LOG K PLOT COMPLETED
```

MG(NO3)2 = N205 + MGO



19 AUG 71

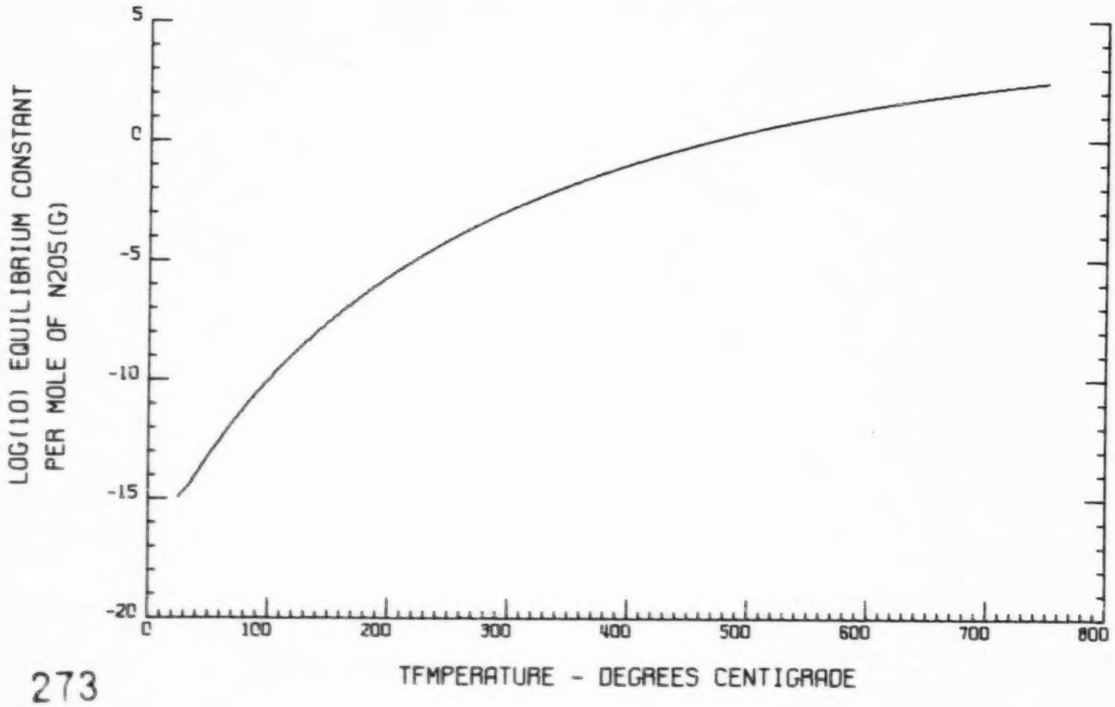
```
8  OCT.  19                         MG(NO3)2 + CO2 I N2O5(G) + MGCO3


      TEMPERATURE             ENTHALPY              ENTROPY                LOG  K
        DEG. C              CAL./GMOLE        CAL./GMOLE/DEG.K

      2.5000+01             2.1695+04            4.4565+00            -1.4928+01
      5.0000+01             3.5178+04            4.8589+01            -1.3171+01
      1.0000+02             3.5027+04            4.8151+01            -9.9907+00
      1.5000+02             3.4906+04            4.7846+01            -7.5708+00
      2.0000+02             3.4755+04            4.7511+01            -5.6696+00
      2.5000+02             3.4559+04            4.7078+01            -4.1397+00
      3.0000+02             3.4234+04            4.6521+01            -2.8862+00
      3.5000+02             3.3823+04            4.5836+01            -1.8447+00
      4.0000+02             3.3297+04            4.5025+01            -9.7007-01
      4.5000+02             3.2647+04            4.4094+01            -2.2956-01
      5.0000+02             3.1868+04            4.3054+01             4.0123-01
      5.5000+02             3.0956+04            4.1912+01             9.4090-01
      6.0000+02             2.9908+04            4.0676+01             1.4039+00
      6.5000+02             2.8721+04            3.9356+01             1.8016+00
      7.0000+02             2.7395+04            3.7957+01             2.1451+00
      7.5000+02             2.5928+04            3.6488+01             2.4360+00

          HR PLOT COMPLETED
          SR PLOT COMPLETED
          LOG K PLOT COMPLETED
```

MG(NO3)2 + CO2 - N2O5(G) + MGCO3



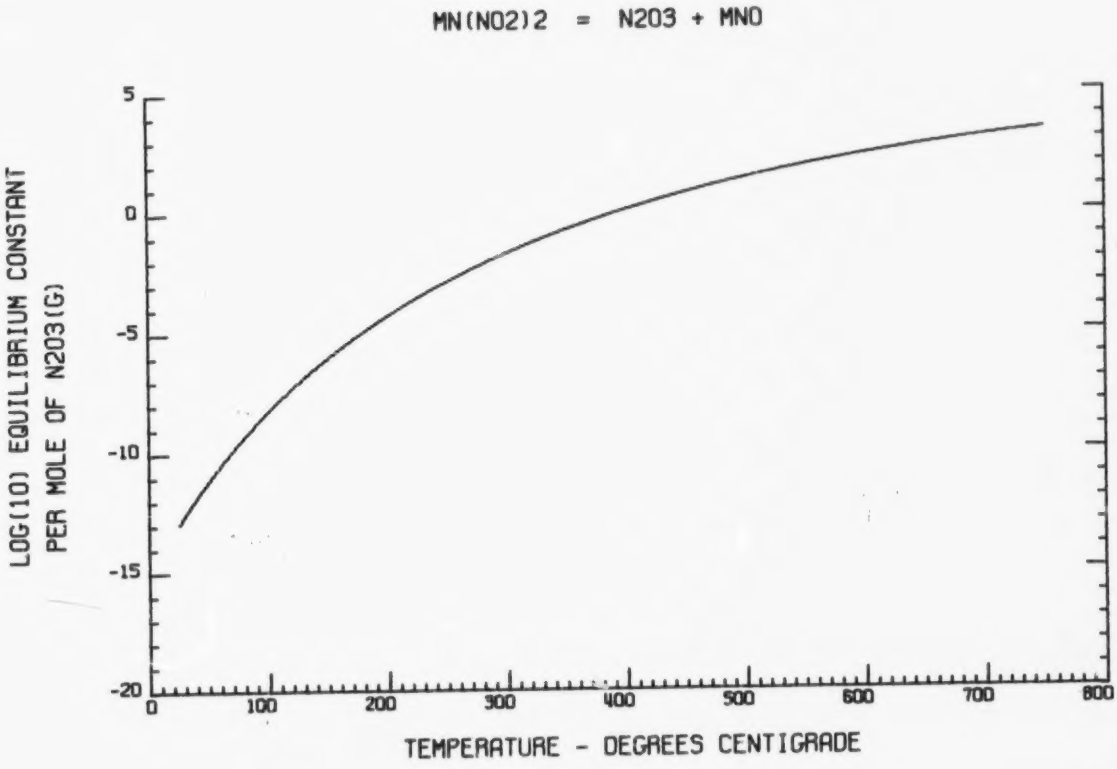
08 OCT 71

```
9 SEPT.  1971                        MN(NO2)2  =  N2O3 + MNO


      TEMPERATURE              ENTHALPY               ENTROPY                LOG  K
       DEG. C                 CAL./GMOLE         CAL./GMOLE/DEG.K

      2.5000+01               3.1881+04              4.7875+01            -1.2905+01
      5.0000+01               3.1906+04              4.7953+01            -1.1097+01
      1.0000+02               3.1969+04              4.8137+01            -8.2030+00
      1.5000+02               3.2011+04              4.8242+01            -5.9892+00
      2.0000+02               3.1999+04              4.8218+01            -4.2422+00
      2.5000+02               3.1915+04              4.8050+01            -2.8312+00
      3.0000+02               3.1746+04              4.7741+01            -1.6709+00
      3.5000+02               3.1482+04              4.7302+01            -7.0333-01
      4.0000+02               3.1119+04              4.6742+01             1.1235-01
      4.5000+02               3.0652+04              4.6074+01             8.0594-01
      5.0000+02               3.0077+04              4.5306+01             1.3997+00
      5.5000+02               2.9393+04              4.4449+01             1.9105+00
      6.0000+02               2.8596+04              4.3511+01             2.3515+00
      6.5000+02               2.7687+04              4.2498+01             2.7332+00
      7.0000+02               2.6663+04              4.1419+01             3.0640+00
      7.5000+02               2.5524+04              4.0278+01             3.3506+00

          HR PLOT COMPLETED
          SR PLOT COMPLETED
          LOG K PLOT COMPLETED
```



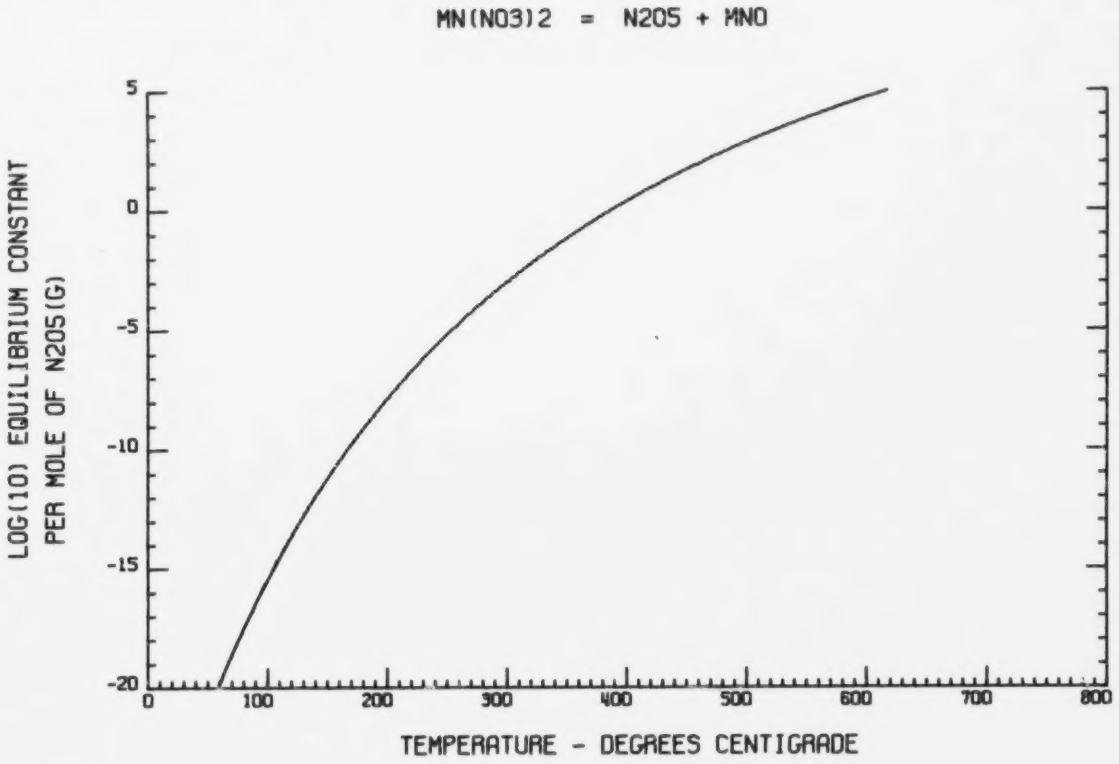
09 SEP 71

```
9 SEPT.  1971                    MN(NO3)2  =  N2O5 + MNO

   TEMPERATURE              ENTHALPY               ENTROPY                   LOG  K
    DEG. C                 CAL./GMOLE          CAL./GMOLE/DEG.K

   2.5000+01               4.8501+04              5.1465+01              -2.4302+01
   5.0000+01               6.1940+04              9.5453+01              -2.1027+01
   1.0000+02               6.1611+04              9.4508+01              -1.5429+01
   1.5000+02               6.1265+04              9.3637+01              -1.1177+01
   2.0000+02               6.0694+04              9.2809+01              -7.8427+00
   2.5000+02               6.0494+04              9.2006+01              -5.1631+00
   3.0000+02               6.0061+04              9.1217+01              -2.9662+00
   3.5000+02               5.9595+04              9.0438+01              -1.1355+00
   4.0000+02               5.9093+04              8.9663+01               4.1055-01
   4.5000+02               5.8555+04              8.8892+01               1.7311+00
   5.0000+02               5.7979+04              8.8123+01               2.8701+00
   5.5000+02               5.7366+04              8.7354+01               3.8604+00
   6.0000+02               5.6714+04              8.6586+01               4.7277+00
   6.5000+02               5.6029+04              8.5818+01               5.4920+00
   7.0000+02               5.5295+04              8.5049+01               6.1691+00
   7.5000+02               5.4527+04              8.4279+01               6.7718+00

        HR PLOT COMPLETED
        SR PLOT COMPLETED
        LOG K PLOT COMPLETED
```



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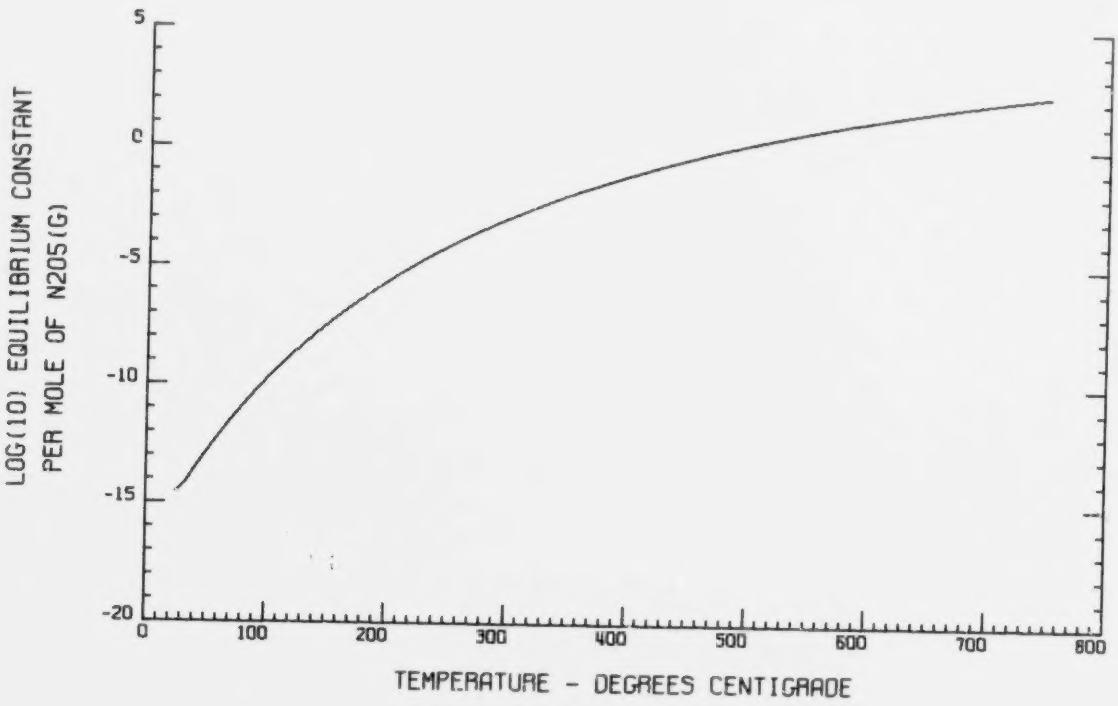
```
8  OCT.  1971                          MN(NO3)2 + CO2  I  N2O5(G) + MNCO3

      TEMPERATURE           ENTHALPY             ENTROPY
        DEG. C            CAL./GMOLE      CAL./GMOLE/DEG.K          LOG  K

      2.5000+01           2.0696+04           2.8345+00         -1.4550+01
      5.0000+01           3.4136+04           4.6827+01         -1.2851+01
      1.0000+02           3.3849+04           4.6001+01         -9.7704+00
      1.5000+02           3.3583+04           4.5332+01         -7.4370+00
      2.0000+02           3.3319+04           4.4742+01         -5.6112+00
      2.5000+02           3.3046+04           4.4193+01         -4.1462+00
      3.0000+02           3.2756+04           4.3665+01         -2.9470+00
      3.5000+02           3.2446+04           4.3147+01         -1.9494+00
      4.0000+02           3.2112+04           4.2631+01         -1.1085+00
      4.5000+02           3.1753+04           4.2116+01         -3.9155-01
      5.0000+02           3.1366+04           4.1600+01          2.2534-01
      5.5000+02           3.0951+04           4.1080+01          7.6042-01
      6.0000+02           3.0509+04           4.0558+01          1.2277+00
      6.5000+02           3.0037+04           4.0033+01          1.6382+00
      7.0000+02           2.9537+04           3.9506+01          2.0005+00
      7.5000+02           2.9009+04           3.8976+01          2.3219+00

          HR PLOT COMPLETED
          SR PLOT COMPLETED
          LOG K PLOT COMPLETED
```

MN(NO3)2 + CO2 - N2O5(G) + MNCO3



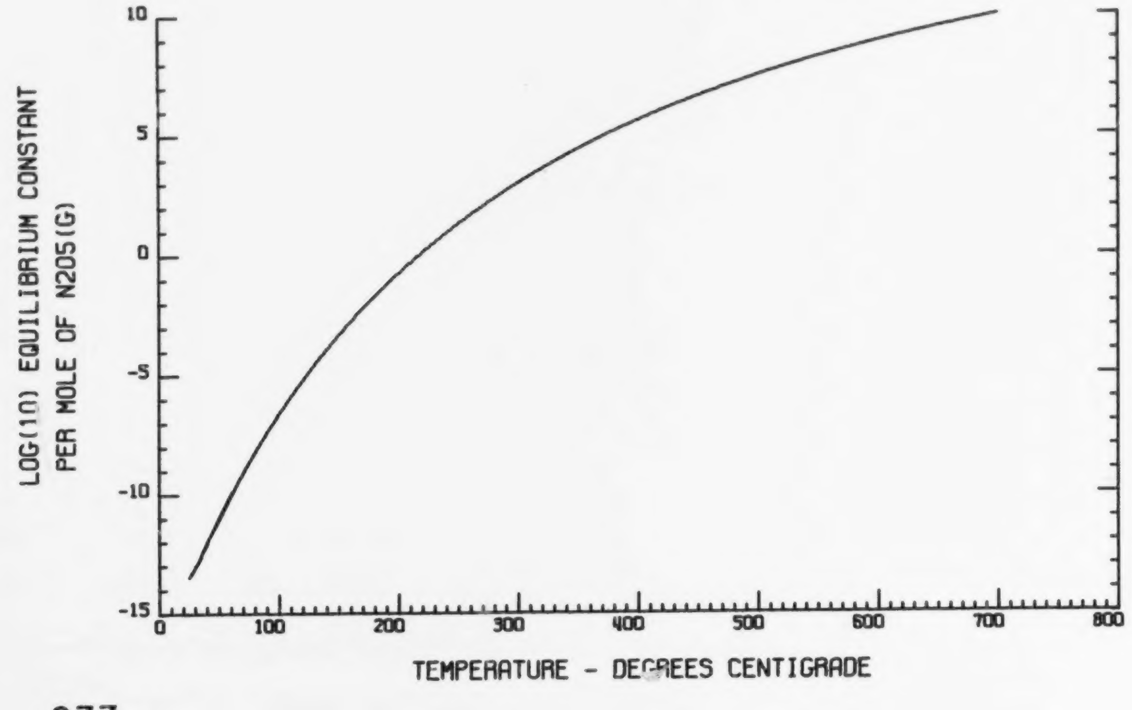
```
9 SEPT.  1971                       2MN(NO3)3  =  3N205 + MN203


     TEMPERATURE              ENTHALPY                ENTROPY                    LOG  K
       DEG. C               CAL./GMOLE          CAL./GMOLE/DEG.K

     2.5000+01               3.4645+04              5.4733+01               -1.3432+01
     5.0000+01               4.0084+04              9.8721+01               -1.0942+01
     1.0000+02               4.7755+04              9.7776+01               -6.5995+00
     1.5000+02               4.7409+04              9.6906+01               -3.3065+00
     2.0000+02               4.7038+04              9.6078+01               -7.2859-01
     2.5000+02               4.6637+04              9.5274+01                1.3393+00
     3.0000+02               4.6205+04              9.4486+01                3.0313+00
     3.5000+02               4.5739+04              9.3706+01                4.4380+00
     4.0000+02               4.5237+04              9.2931+01                5.6232+00
     4.5000+02               4.4698+04              9.2160+01                6.6327+00
     5.0000+02               4.4123+04              9.1390+01                7.5006+00
     5.5000+02               4.3509+04              9.0622+01                8.2553+00
     6.0000+02               4.2857+04              8.9853+01                8.9099+00
     6.5000+02               4.2167+04              8.9084+01                9.4863+00
     7.0000+02               4.1437+04              8.8315+01                9.9949+00
     7.5000+02               4.0669+04              8.7545+01                1.0446+01

         HR PLOT COMPLETED
         SR PLOT COMPLETED
         LOG K PLOT COMPLETED
```

2MN(NO3)3 = 3N205 + MN203



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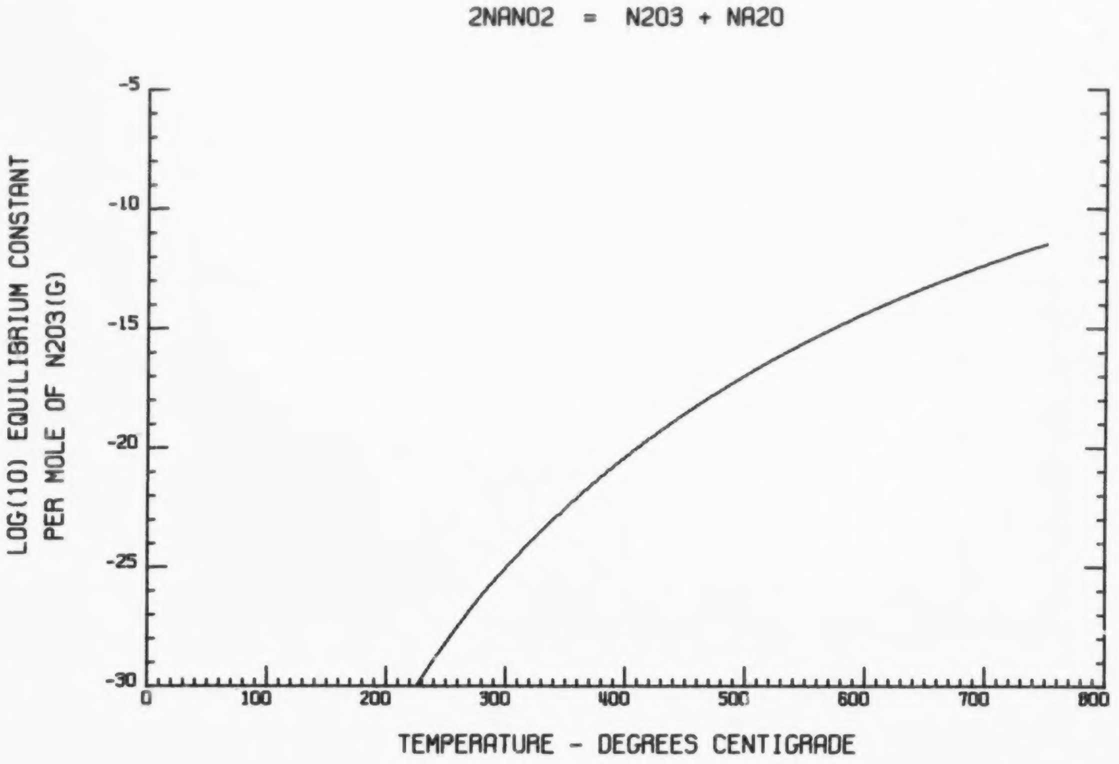
```
9 SEPT.  1971                       2NANO2  =  N2O3 + NA2O


   TEMPERATURE              ENTHALPY               ENTROPY                LOG  K
    DEG. C                 CAL./GMOLE         CAL./GMOLE/DEG.K

    2.5000+01              8.8370+04              4.0216+01             -5.5983+01
    5.0000+01              8.8394+04              4.0292+01             -5.0971+01
    1.0000+02              8.8456+04              4.0472+01             -4.2959+01
    1.5000+02              8.8497+04              4.0575+01             -3.6856+01
    2.0000+02              8.7886+04              3.9174+01             -3.2031+01
    2.5000+02              8.7801+04              3.9004+01             -2.8153+01
    3.0000+02              8.2661+04              2.9726+01             -2.5021+01
    3.5000+02              8.2396+04              2.9285+01             -2.2496+01
    4.0000+02              8.2031+04              2.8723+01             -2.0354+01
    4.5000+02              8.1562+04              2.8052+01             -1.8518+01
    5.0000+02              8.0986+04              2.7282+01             -1.6929+01
    5.5000+02              8.0299+04              2.6422+01             -1.5544+01
    6.0000+02              7.9501+04              2.5481+01             -1.4329+01
    6.5000+02              7.8589+04              2.4467+01             -1.3258+01
    7.0000+02              7.7563+04              2.3385+01             -1.2308+01
    7.5000+02              7.6421+04              2.2241+01             -1.1463+01

         HR PLOT COMPLETED
         SR PLOT COMPLETED
         LOG K PLOT COMPLETED
```


2NANO2 = N2O3 + NA2O

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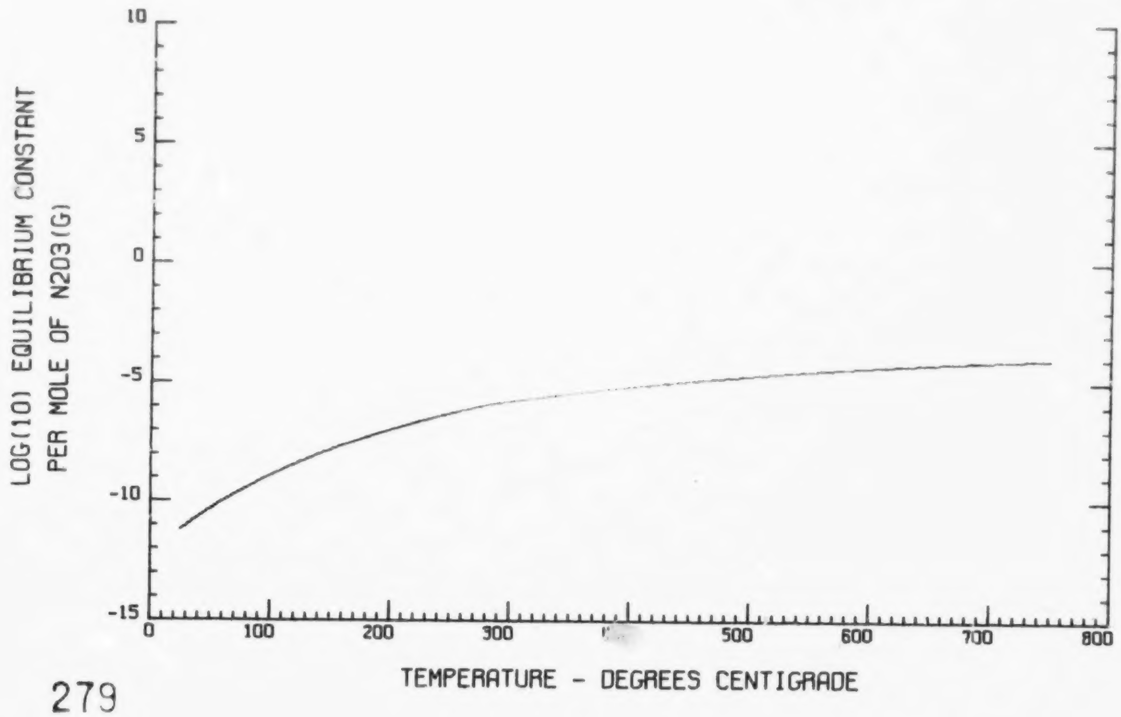
```
8 OCT. 1971                    2NANO2 + CO2  I  N2O3(G) + NA2CO3

    TEMPERATURE           ENTHALPY              ENTROPY                LOG  K
      DEG. C             CAL./GMOLE          CAL./GMOLE/DEG.K

    2.5000+01            1.5531+04             8.8114-01             -1.1191+01
    5.0000+01            1.5563+04             9.8133-01             -1.0310+01
    1.0000+02            1.5664+04             1.2720+00             -8.8957+00
    1.5000+02            1.5801+04             1.6152+00             -7.8074+00
    2.0000+02            1.5362+04             5.9667-01             -6.9651+00
    2.5000+02            1.5537+04             9.4711-01             -6.2832+00
    3.0000+02            1.0753+04            -7.6822+00             -5.7788+00
    3.5000+02            1.0945+04            -7.3605+00             -5.4470+00
    4.0000+02            1.1143+04            -7.0544+00             -5.1594+00
    4.5000+02            1.1346+04            -6.7641+00             -4.9070+00
    5.0000+02            1.1371+04            -6.7247+00             -4.6838+00
```

2NANO2 + CO2 - N2O3(G) + NA2CO3



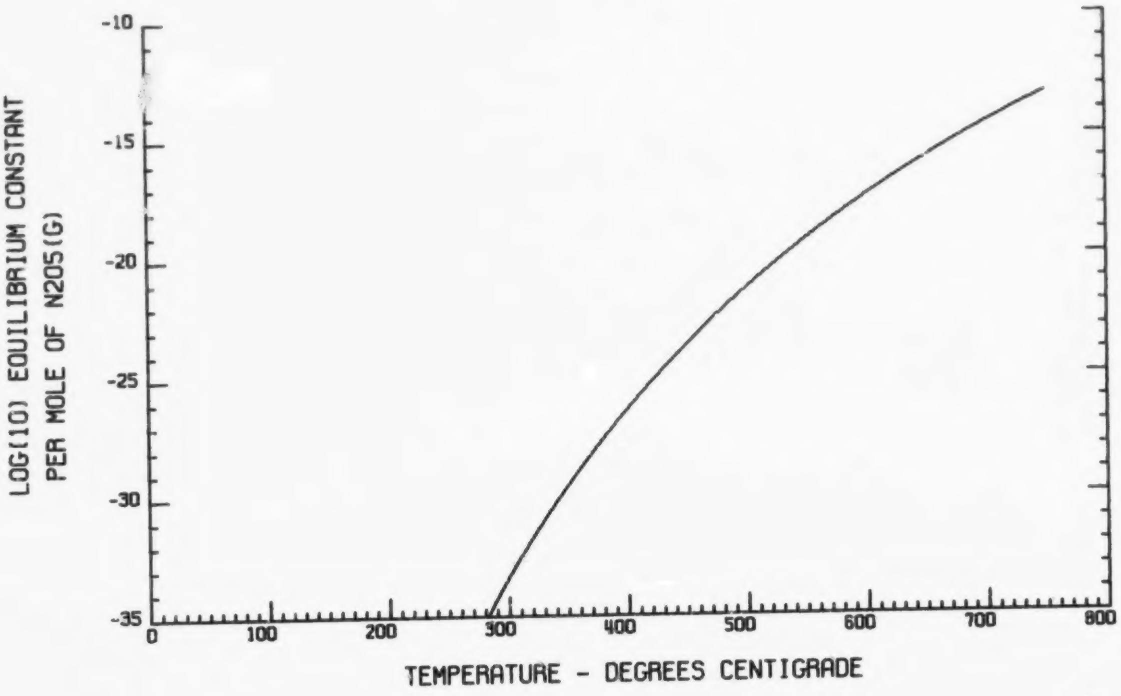
08 OCT 71

19 AUG. 1971

2NANO3 = N205 +NA20

TEMPERATURE DEG. C	ENTHALPY CAL./GMOLE	ENTROPY CAL./GMOLE/DEG.K	LOG K
2.5000+01	1.2353+05	4.4186+01	-8.0886+01
5.0000+01	1.3693+05	8.6061+01	-7.3357+01
1.0000+02	1.3649+05	8.6794+01	-6.0968+01
1.5000+02	1.3595+05	8.5385+01	-5.1540+01
2.0000+02	1.3521+05	8.3774+01	-4.4140+01
2.5000+02	1.3430+05	8.1949+01	-3.8191+01
3.0000+02	1.3097+05	7.5679+01	-3.3355+01
3.5000+02	1.2239+05	6.1128+01	-2.9562+01
4.0000+02	1.2123+05	5.9336+01	-2.6585+01
4.5000+02	1.2010+05	5.7721+01	-2.3680+01
5.0000+02	1.1901+05	5.6261+01	-2.1344+01
5.5000+02	1.1795+05	5.4930+01	-1.9309+01
6.0000+02	1.1691+05	5.3710+01	-1.7524+01
6.5000+02	1.1590+05	5.2566+01	-1.5946+01
7.0000+02	1.1492+05	5.1547+01	-1.4542+01
7.5000+02	1.1396+05	5.0563+01	-1.3286+01

2NANO3 = N205 +NA20

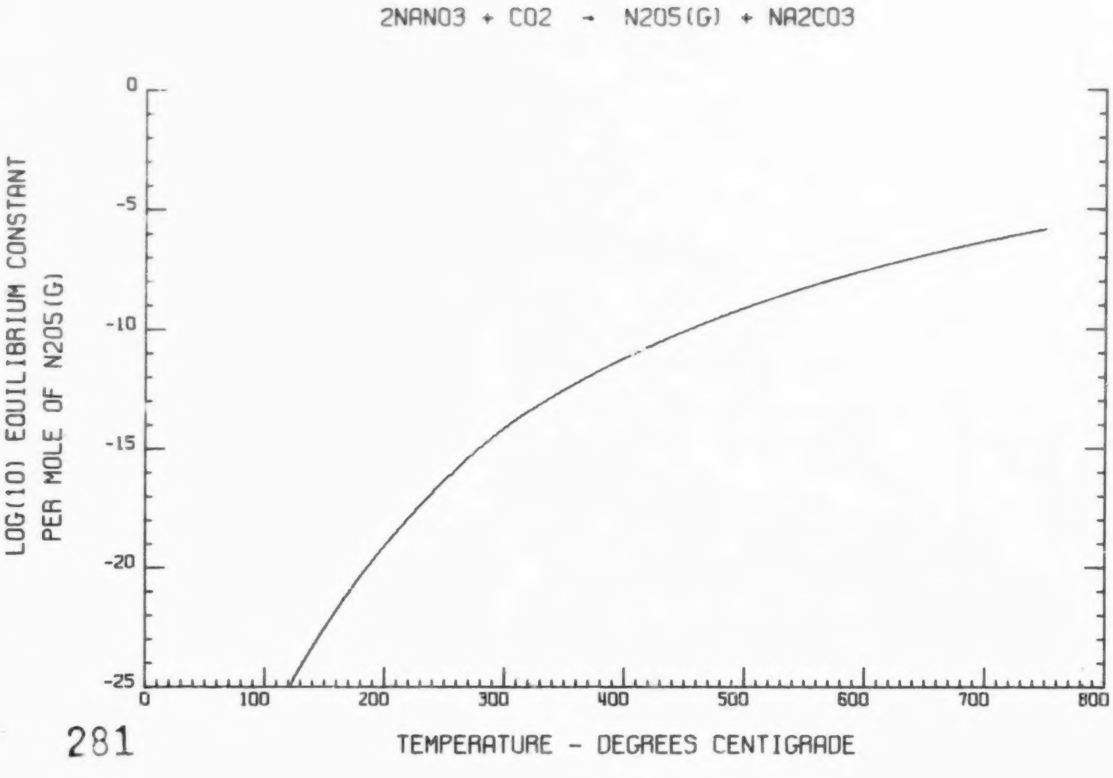


```
8  OCT.  1971                    2NANO3 + CO2  =  N2O5(G) + NA2CO3

     TEMPERATURE              ENTHALPY              ENTROPY               LOG  K
      DEG. C                CAL./GMOLE         CAL./GMOLE/DEG.K

     2.5000+01              5.0691+04             4.8511+00            -3.6095+01
     5.0000+01              6.4102+04             4.8750+01            -3.2696+01
     1.0000+02              6.3700+04             4.7594+01            -2.6904+01
     1.5000+02              6.3234+04             4.6425+01            -2.2511+01
     2.0000+02              6.2603+04             4.5197+01            -1.9074+01
     2.5000+02              6.2033+04             4.3892+01            -1.6521+01
     3.0000+02              5.9062+04             3.8470+01            -1.4112+01
     3.5000+02              5.0939+04             2.4483+01            -1.2513+01
     4.0000+02              5.0339+04             2.3556+01            -1.1194+01
     4.5000+02              4.9585+04             2.2905+01            -1.0070+01
     5.0000+02              4.9395+04             2.2254+01            -9.0984+00
     5.5000+02              4.8542+04             2.1185+01            -8.2577+00
     6.0000+02              4.7770+04             2.0273+01            -7.5255+00
     6.5000+02              4.7076+04             1.9500+01            -6.8827+00
     7.0000+02              4.6459+04             1.8849+01            -6.3159+00
     7.5000+02              4.5919+04             1.8308+01            -5.8070+00

         HR PLOT COMPLETED
         SR PLOT COMPLETED
         LOG K PLOT COMPLETED
```



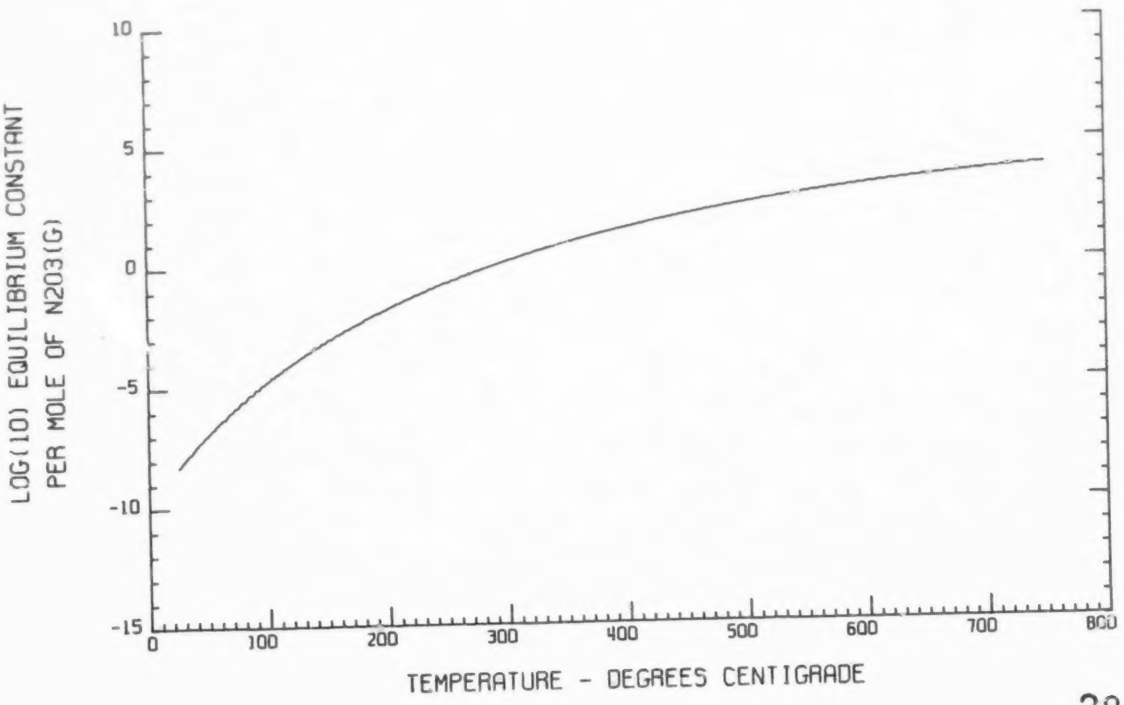
08 OCT 71

```
9 SEPT.  1971                         NI(NO2)2  =  N203 + NIO

                                                                                    LOG  K
       TEMPERATURE              ENTHALPY                 ENTROPY
         DEG. C               CAL./GMOLE           CAL./GMOLE/DEG.K
                                                                                -8.2585+00
        2.5000+01             2.3936+04               4.2488+01                 -6.9014+00
        5.0000+01             2.3936+04               4.2490+01                 -4.7314+00
        1.0000+02             2.3967+04               4.2577+01                 -3.0715+00
        1.5000+02             2.4017+04               4.2702+01                 -1.7592+00
        2.0000+02             2.4071+04               4.2823+01                 -6.9555-01
        2.5000+02             2.4119+04               4.2920+01                  1.8024-01
        3.0000+02             2.3926+04               4.2568+01                  9.0817-01
        3.5000+02             2.3638+04               4.2088+01                  1.5194+00
        4.0000+02             2.3251+04               4.1492+01                  2.0360+00
        4.5000+02             2.2762+04               4.0791+01                  2.4755+00
        5.0000+02             2.2166+04               3.9996+01                  2.8501+00
        5.5000+02             2.1462+04               3.9115+01                  3.1705+00
        6.0000+02             2.0649+04               3.8156+01                  3.4444+00
        6.5000+02             1.9725+04               3.7128+01                  3.6782+00
        7.0000+02             1.8689+04               3.6035+01                  3.8772+00
        7.5000+02             1.7541+04               3.4985+01

            HR PLOT COMPLETED
            SR PLOT COMPLETED
            LOG K PLOT COMPLETED
```

NI(NO2)2 = N203 + NIO



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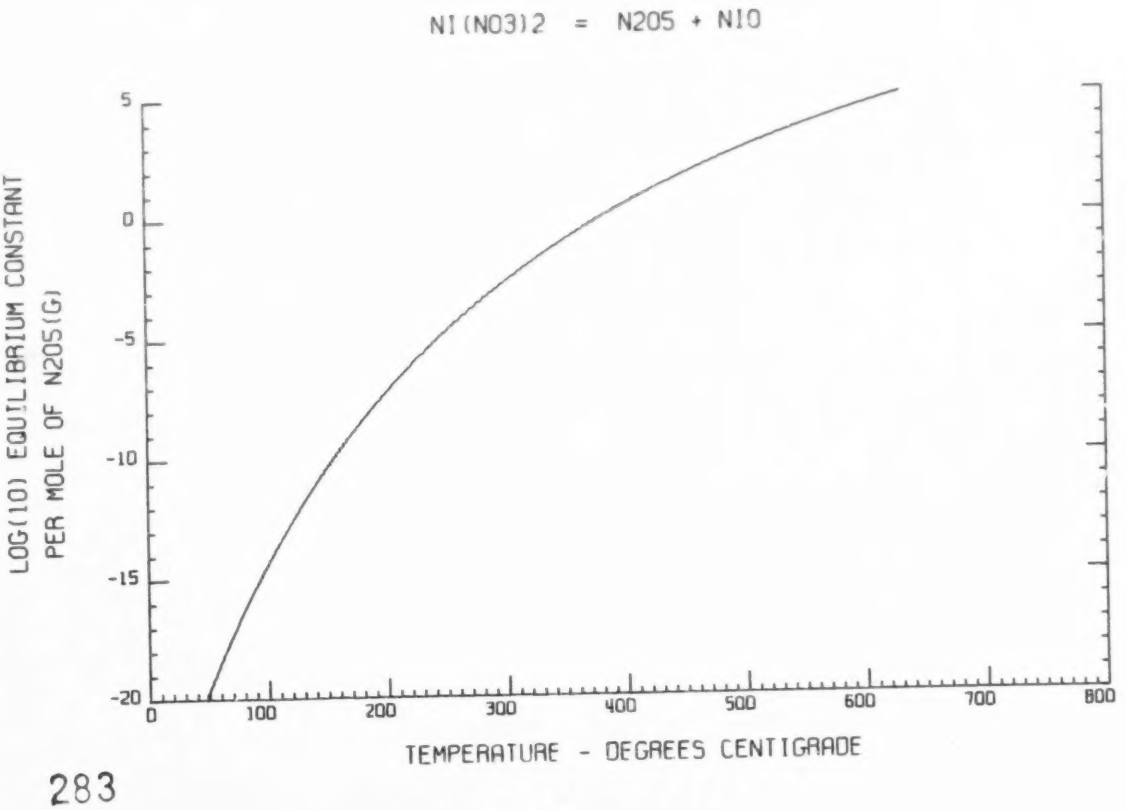
```
9 SEPT.  1971                      NI(NO3)2  =  N2O5 + NIO


   TEMPERATURE           ENTHALPY              ENTROPY                 LOG  K
     DEG. C            CAL./GMOLE       CAL./GMOLE/DEG.K

   2.5000+01           4.4636+04          4.6078+01              -2.2646+01
   5.0000+01           5.8050+04          8.9989+01              -1.9591+01
   1.0000+02           5.7688+04          8.8947+01              -1.4346+01
   1.5000+02           5.7350+04          8.8095+01              -1.0366+01
   2.0000+02           5.7044+04          8.7411+01              -7.2442+00
   2.5000+02           5.6776+04          8.6673+01              -4.7320+00
   3.0000+02           5.6320+04          8.6040+01              -2.6710+00
   3.5000+02           5.5829+04          8.5219+01              -9.551[illegible]01
   4.0000+02           5.5303+04          8.4408+01               4.92[illegible]1
   4.5000+02           5.4742+04          8.3604+01               1.72[illegible]
   5.0000+02           5.4145+04          8.2806+01               2.792[illegible]
   5.5000+02           5.3512+04          8.2013+01               3.716[illegible]00
   6.0000+02           5.2643+04          8.1225+01               4.5249+00
   6.5000+02           5.2138+04          8.0439+01               5.2366+00
   7.0000+02           5.1396+04          7.9657+01               5.8664+00
   7.5000+02           5.0618+04          7.8877+01               6.4262+00

       HR PLOT COMPLETED
       SR PLOT COMPLETED
       LOG K PLOT COMPLETED
```



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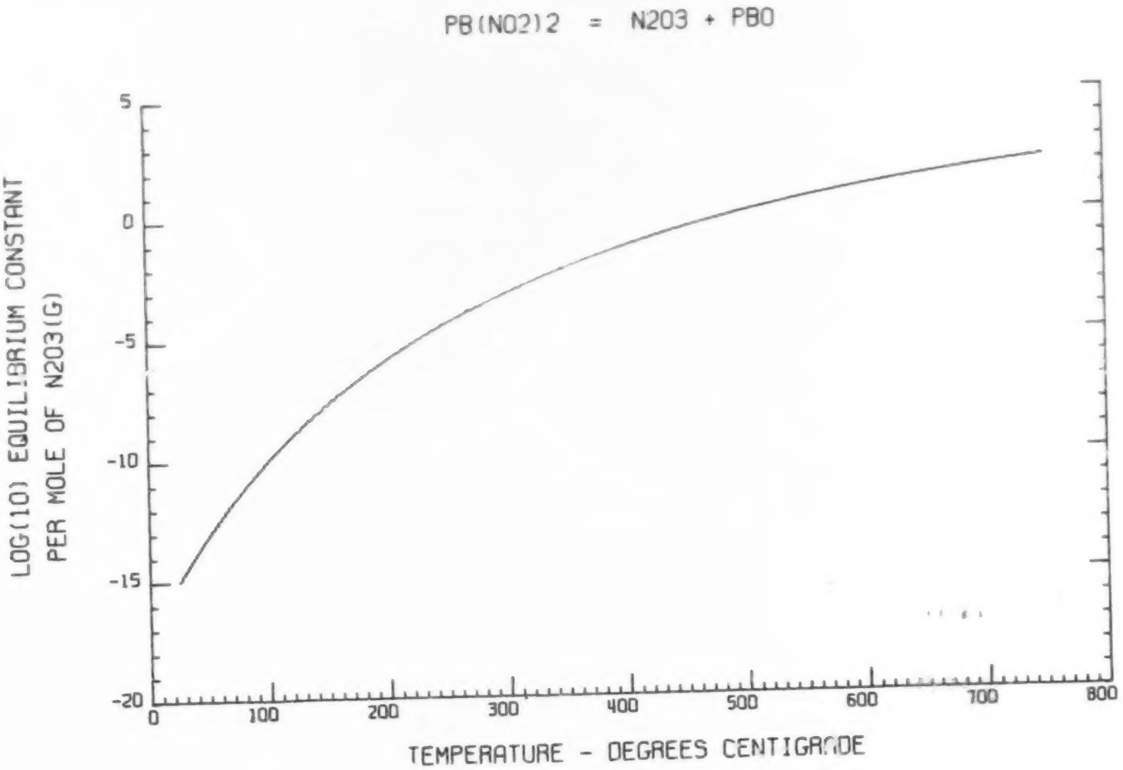
```
9 SEPT.  1971                    PB(NO2)2  =  N2O3 + PBO

                                                                              LOG  K
                                                        ENTROPY
  TEMPERATURE             ENTHALPY               CAL./GMOLE/DEG.K
   DEG. C                CAL./GMOLE                                        -1.4960+01
                          3.3533+04               4.4010+01                -1.3056+01
  2.5000+01               3.3558+04               4.4089+01                -1.0015+01
  5.0000+01               3.3621+04               4.4272+01                -7.6866+00
  1.0000+02               3.3663+04               4.4378+01                -5.8497+00
  1.5000+02               3.3651+04               4.4353+01                -4.3656+00
  2.0000+02               3.3567+04               4.4185+01                -3.1453+00
  2.5000+02               3.3398+04               4.3877+01                -2.1272+00
  3.0000+02               3.3134+04               4.3437+01                -1.2665+00
  3.5000+02               3.2771+04               4.2876+01                -5.3786-01
  4.0000+02               3.2304+04               4.2209+01                 8.8124-02
  4.5000+02               3.1729+04               4.1441+01                 5.2726-01
  5.0000+02               3.1044+04               4.0584+01                 1.0934+00
  5.5000+02               3.0248+04               3.9646+01                 1.4976+00
  6.0000+02               2.9339+04               3.8634+01                 1.8484+00
  6.5000+02               2.8315+04               3.7554+01                 2.1531+00
  7.0000+02               2.7176+04               3.6413+01
  7.5000+02

      HR PLOT COMPLETED
      SR PLOT COMPLETED
      LOG K PLOT COMPLETED
```



PB(NO2)2 = N203 + PBO

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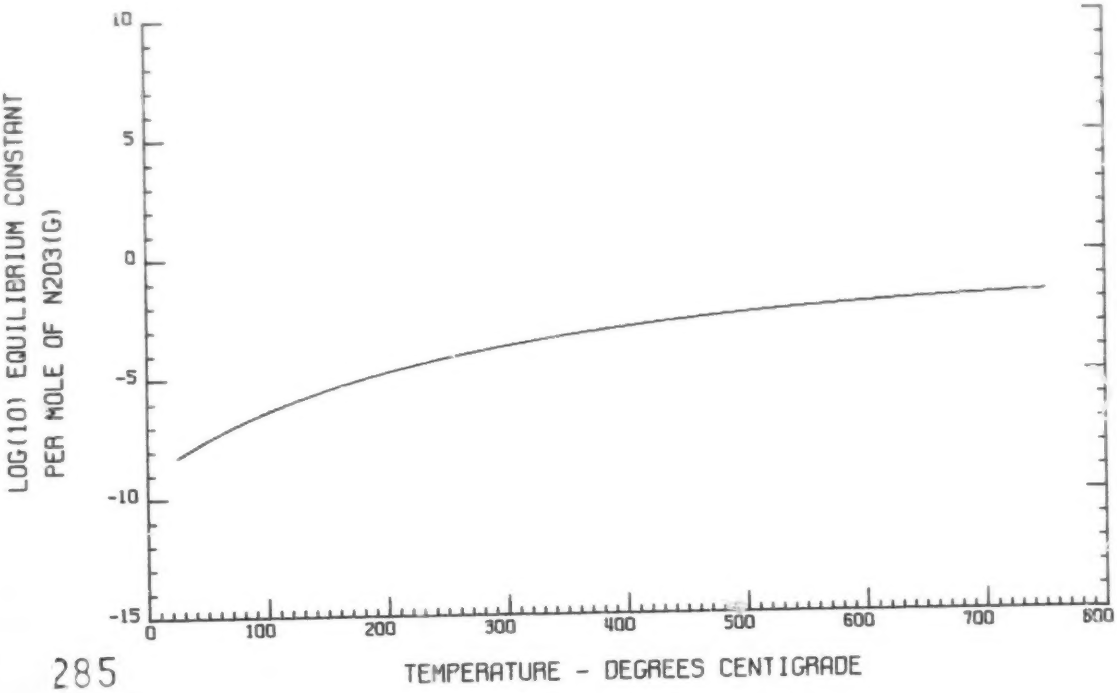
```
11  OCT.  1971                PB(NO2)2 + CO2  I  N2O3(G) + PBCO3

     TEMPERATURE              ENTHALPY                ENTROPY              LOG  K
       DEG. C               CAL./GMOLE         CAL./GMOLE/DEG.K

                                                  4.8428+00            -8.2353+00
     2.5000+01               1.2680+04            4.8988+00            -7.5160+00
     5.0000+01               1.2697+04            5.2050+00            -6.3613+00
     1.0000+02               1.2804+04            5.5535+00            -5.4707+00
     1.5000+02               1.2943+04            5.8250+00            -4.7610+00
     2.0000+02               1.3064+04            5.9752+00            -4.1825+00
     2.5000+02               1.3139+04            5.9911+00            -3.7034+00
     3.0000+02               1.3147+04            5.8736+00            -3.3020+00
     3.5000+02               1.3076+04            5.6299+00            -2.9632+00
     4.0000+02               1.2917+04            5.2691+00            -2.6759+00
     4.5000+02               1.2665+04            4.8009+00            -2.4316+00
     5.0000+02               1.2314+04            4.2349+00            -2.2238+00
     5.5000+02               1.1862+04            3.5799+00            -2.0475+00
     6.0000+02               1.1306+04            2.8439+00            -1.8985+00
     6.5000+02               1.0645+04            2.0343+00            -1.7735+00
     7.0000+02               9.8771+03            1.1576+00            -1.6697+00
     7.5000+02               9.0018+03

          HR PLOT COMPLETED
          SR PLOT COMPLETED
          LOG K PLOT COMPLETED
```

PB(NO2)2 + CO2 - N2O3(G) + PBCO3



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08 OCT 71

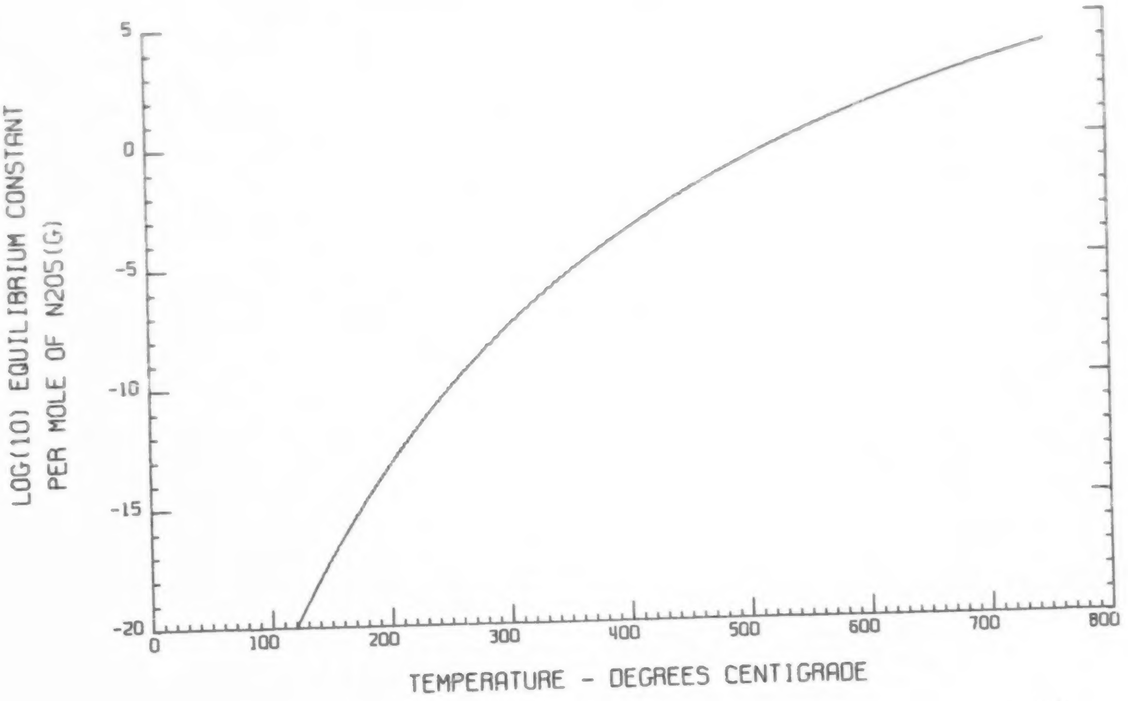
```
9 SEPT.  1971                       PB(NO3)2  =  N2O5 + PBO

                                                                        LOG  K
   TEMPERATURE          ENTHALPY              ENTROPY
     DEG. C            CAL./GMOLE        CAL./GMOLE/DEG.K

   2.5000+01           5.8333+04            4.7600+01           -3.2355+01
   5.0000+01           7.1772+04            9.1589+01           -2.8520+01
   1.0000+02           7.1443+04            9.0643+01           -2.2031+01
   1.5000+02           7.1097+04            8.9773+01           -1.7099+01
   2.0000+02           7.0726+04            8.8944+01           -1.3228+01
   2.5000+02           7.0325+04            8.8141+01           -1.0115+01
   3.0000+02           6.9893+04            8.7352+01           -7.5595+00
   3.5000+02           6.9427+04            8.6573+01           -5.4281+00
   4.0000+02           6.8925+04            8.5798+01           -3.6259+00
   4.5000+02           6.8386+04            8.5027+01           -2.0847+00
   5.0000+02           6.7811+04            8.4258+01           -7.5360-01
   5.5000+02           6.7197+04            8.3489+01            4.0555-01
   6.0000+02           6.6546+04            8.2721+01            1.4223+00
   6.5000+02           6.5855+04            8.1952+01            2.3199+00
   7.0000+02           6.5126+04            8.1183+01            3.1165+00
   7.5000+02           6.4358+04            8.0414+01            3.8271+00

      HR PLOT COMPLETED
      SR PLOT COMPLETED
      LOG K PLOT COMPLETED
```

PB(NO3)2 = N2O5 + PBO



09 SEP 71

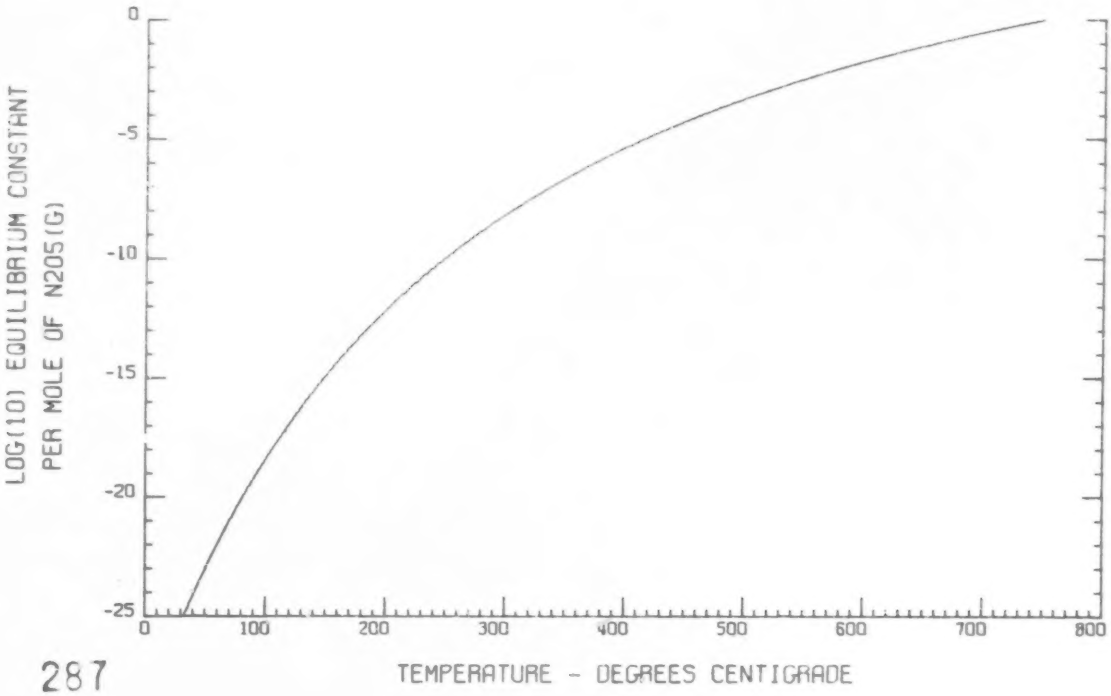
```
11  OCT.  1971                    PB(NO3)2 + CO2 I N205(G) + PBCO3

     TEMPERATURE              ENTHALPY               ENTROPY                  LOG  K
       DEG. C               CAL./GMOLE         CAL./GMOLE/DEG.K

     2.5000+01              3.7480+04             8.4328+00              -2.5628+01
     5.0000+01              5.0911+04             5.2398+01              -2.2978+01
     1.0000+02              5.0626+04             5.1576+01              -1.8377+01
     1.5000+02              5.0376+04             5.0948+01              -1.4883+01
     2.0000+02              5.0138+04             5.0416+01              -1.2140+01
     2.5000+02              4.9897+04             4.9931+01              -9.9315+00
     3.0000+02              4.9642+04             4.9467+01              -8.1176+00
     3.5000+02              4.9368+04             4.9009+01              -6.6029+00
     4.0000+02              4.9071+04             4.8550+01              -5.3207+00
     4.5000+02              4.8748+04             4.8087+01              -4.2227+00
     5.0000+02              4.8396+04             4.7617+01              -3.2735+00
     5.5000+02              4.8015+04             4.7140+01              -2.4455+00
     6.0000+02              4.7604+04             4.6655+01              -1.7186+00
     6.5000+02              4.7162+04             4.6163+01              -1.0762+00
     7.0000+02              4.6688+04             4.5664+01              -5.0535-01
     7.5000+02              4.6184+04             4.5158+01               4.3202-03

         HR PLOT COMPLETED
         SR PLOT COMPLETED
         LOG K PLOT COMPLETED
```

PB(NO3)2 + CO2 → N2O5(G) + PBCO3



08 OCT 71

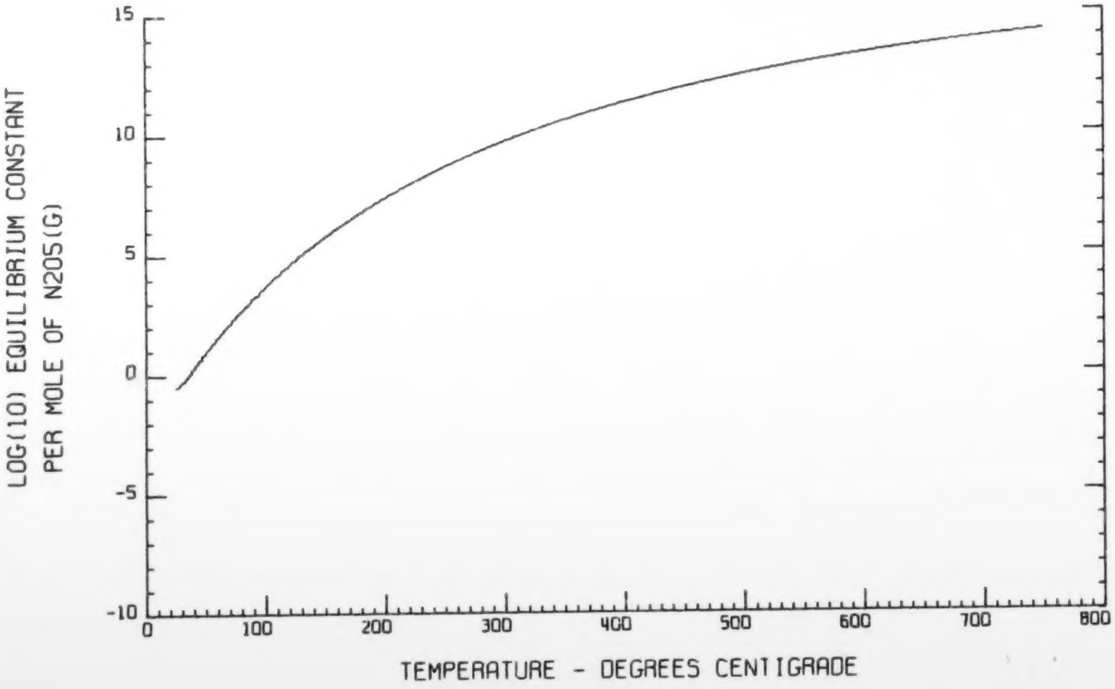
```
9 SEPT.  1971                    SN(NO3)4  =  2N205 + SNO2

     TEMPERATURE            ENTHALPY            ENTROPY              LOG  K
      DEG. C              CAL./GMOLE       CAL./GMOLE/DEG.K

     2.5000+01            1.6953+04           5.4502+01          -5.1536-01
     5.0000+01            3.0392+04           9.8490+01           9.7123-01
     1.0000+02            3.0063+04           9.7544+01           3.7110+00
     1.5000+02            2.9717+04           9.6674+01           5.7800+00
     2.0000+02            2.9346+04           9.5846+01           7.3921+00
     2.5000+02            2.8945+04           9.5042+01           8.6791+00
     3.0000+02            2.8513+04           9.4253+01           9.7264+00
     3.5000+02            2.8046+04           9.3473+01           1.0592+01
     4.0000+02            2.7544+04           9.2699+01           1.1316+01
     4.5000+02            2.7233+04           9.2260+01           1.1933+01
     5.0000+02            2.6657+04           9.1490+01           1.2459+01
     5.5000+02            2.6043+04           9.0721+01           1.2912+01
     6.0000+02            2.5392+04           8.9953+01           1.3303+01
     6.5000+02            2.4701+04           8.9184+01           1.3643+01
     7.0000+02            2.3972+04           8.6415+01           1.3939+01
     7.5000+02            2.3203+04           8.7645+01           1.4198+01

          HR PLOT COMPLETED
          SR PLOT COMPLETED
          LOG K PLOT COMPLETED
```

SN(NO3)4 = 2N205 + SNO2



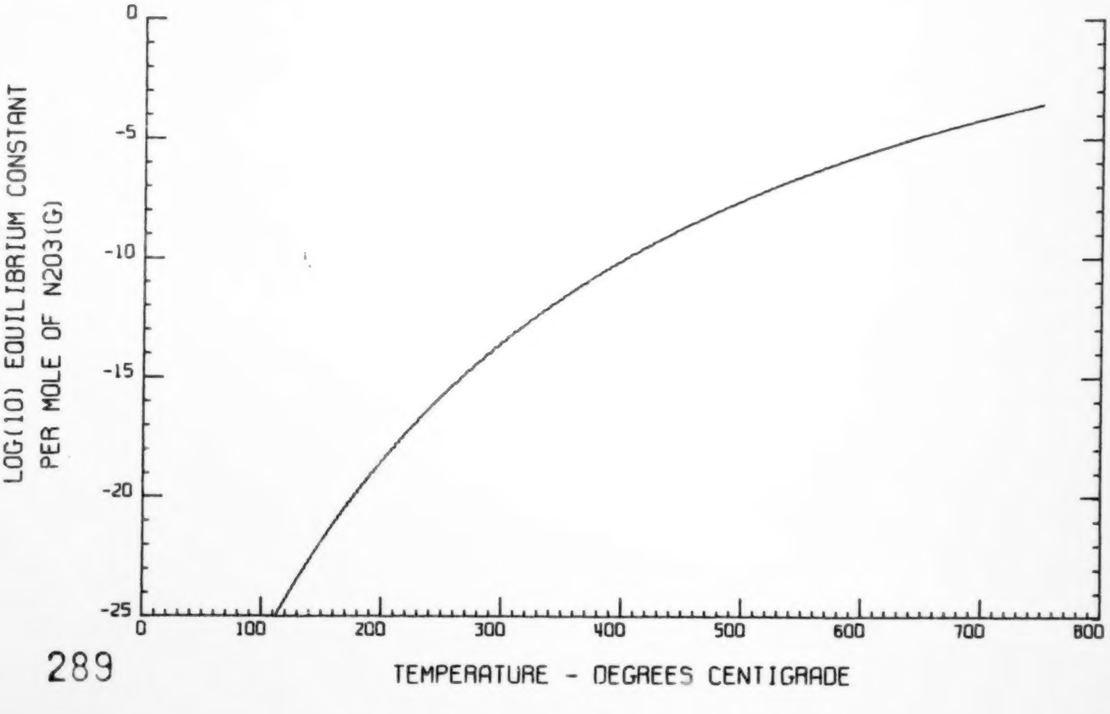
```
9 SEPT.  1971                         SR(NO2)2  =  N2O3 + SRO


        TEMPERATURE                  ENTHALPY                  ENTROPY                   LOG  K
         DEG. C                     CAL./GMOLE           CAL./GMOLE/DEG.K

        2.5000+01                   6.1264+04                 4.4906+01               -3.5090+01
        5.0000+01                   6.1289+04                 4.4985+01               -3.1616+01
        1.0000+02                   6.1352+04                 4.5168+01               -2.6060+01
        1.5000+02                   6.1394+04                 4.5274+01               -2.1812+01
        2.0000+02                   6.1382+04                 4.5249+01               -1.8462+01
        2.5000+02                   6.1298+04                 4.5081+01               -1.5754+01
        3.0000+02                   6.1129+04                 4.4773+01               -1.3523+01
        3.5000+02                   6.0865+04                 4.4334+01               -1.1656+01
        4.0000+02                   6.0502+04                 4.3774+01               -1.0075+01
        4.5000+02                   6.0035+04                 4.3106+01               -8.7223+00
        5.0000+02                   5.9460+04                 4.2338+01               -7.5543+00
        5.5000+02                   5.8776+04                 4.1481+01               -6.5390+00
        6.0000+02                   5.7980+04                 4.0543+01               -5.6513+00
        6.5000+02                   5.7070+04                 3.9531+01               -4.8712+00
        7.0000+02                   5.6047+04                 3.8451+01               -4.1831+00
        7.5000+02                   5.4908+04                 3.7310+01               -3.5741+00

              HR PLOT COMPLETED
              SR PLOT COMPLETED
              LOG K PLOT COMPLETED
```

SR(NO2)2 = N2O3 + SRO



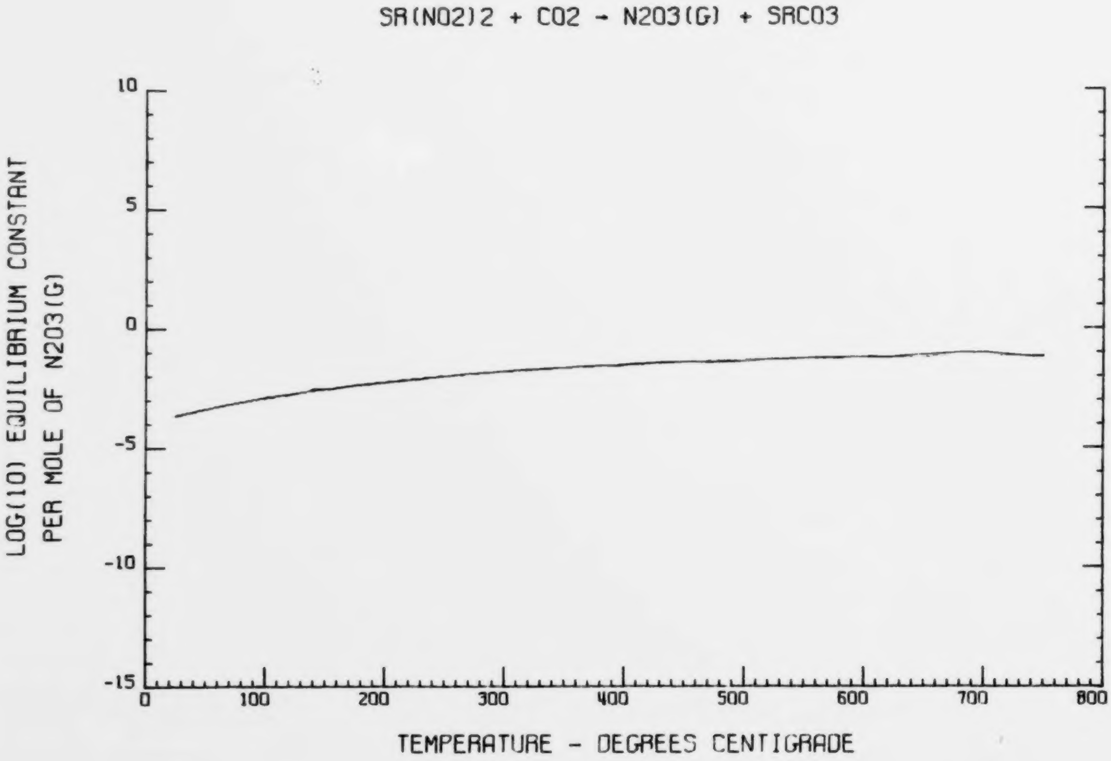
09 SEP 71

```
11  OCT.  1971                  SR(NO2)2 + CO2 I N2O3(G) + SRCO3

      TEMPERATURE              ENTHALPY              ENTROPY                 LOG  K
       DEG. C                CAL./GMOLE          CAL./GMOLE/DEG.K

      2.5000+01              5.0293+03             2.4404-01             -3.6330+00
      5.0000+01              5.0682+03             3.6874-01             -3.3468+00
      1.0000+02              5.1771+03             6.8153-01             -2.8830+00
      1.5000+02              5.2604+03             9.4186-01             -2.5212+00
      2.0000+02              5.3423+03             1.0813+00             -2.2312+00
      2.5000+02              5.3412+03             1.0803+00             -1.9951+00
      3.0000+02              5.2632+03             9.3902-01             -1.8016+00
      3.5000+02              5.0990+03             6.6537-01             -1.6428+00
      4.0000+02              4.8423+03             2.7009-01             -1.5130+00
      4.5000+02              4.4888+03            -2.3568-01             -1.4080+00
      5.0000+02              4.0354+03            -8.4126-01             -1.3245+00
      5.5000+02              3.4798+03            -1.5368+00             -1.2597+00
      6.0000+02              2.8207+03            -2.3136+00             -1.2116+00
      6.5000+02              2.0569+03            -3.1637+00             -1.1783+00
      7.0000+02              1.1878+03            -4.0800+00             -1.1584+00
      7.5000+02              2.1299+02            -5.0564+00             -1.1505+00

          HR PLOT COMPLETED
          SR PLOT COMPLETED
          LOG K PLOT COMPLETED
```

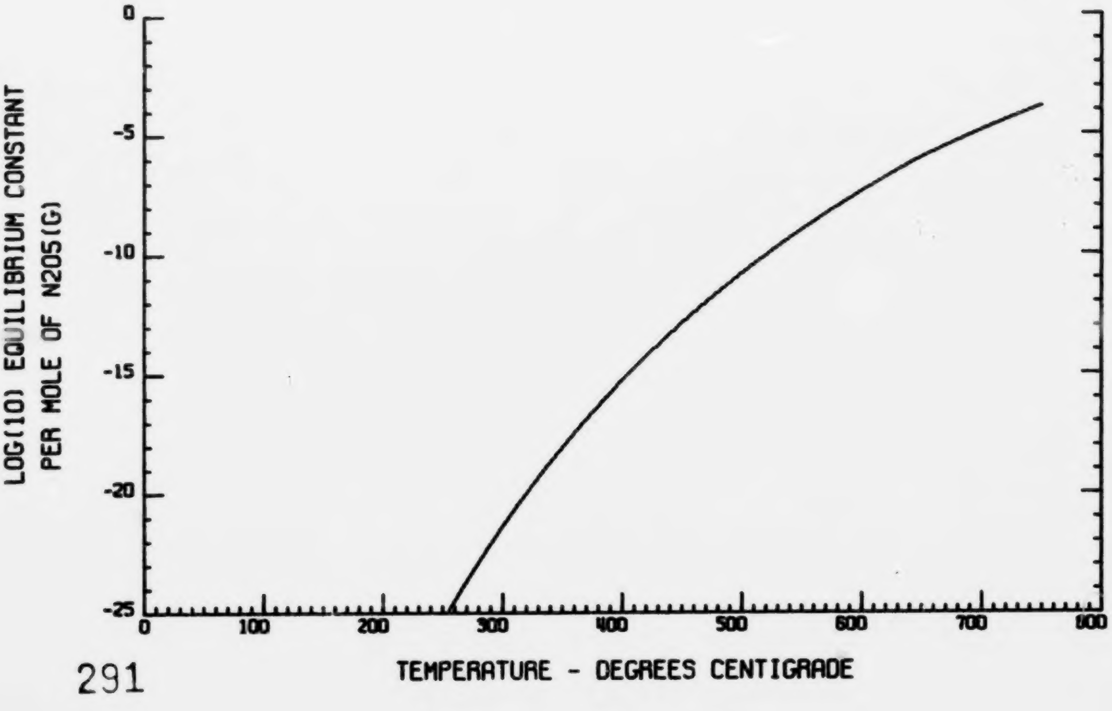


08 OCT 71

SR(NO3)2 = N2O5 +SRO

TEMPERATURE DEG. C	ENTHALPY CAL./GMOLE	ENTROPY CAL./GMOLE/DEG.K	LOG K
2.5000+01	9.5764+04	4.9296+01	-5.9418+01
5.0000+01	1.0523+05	9.3382+01	-5.3462+01
1.0000+02	1.0902+05	9.2772+01	-4.3574+01
1.5000+02	1.0885+05	9.2291+01	-3.6036+01
2.0000+02	1.0662+05	9.1829+01	-3.0102+01
2.5000+02	1.0638+05	9.1337+01	-2.5312+01
3.0000+02	1.0608+05	9.0793+01	-2.1368+01
3.5000+02	1.0772+05	9.0196+01	-1.8066+01
4.0000+02	1.0729+05	8.9526+01	-1.5266+01
4.5000+02	1.0676+05	8.8865+01	-1.2865+01
5.0000+02	1.0620+05	8.8023+01	-1.0781+01
5.5000+02	1.0553+05	8.7191+01	-8.9636+00
6.0000+02	1.0479+05	8.6309+01	-7.3646+00
6.5000+02	9.3299+04	7.3777+01	-5.9633+00
7.0000+02	9.2379+04	7.2608+01	-4.8340+00
7.5000+02	9.1373+04	7.1795+01	-3.8255+00

SR(NO3)2 = N2O5 +SRO



TEMPERATURE - DEGREES CENTIGRADE

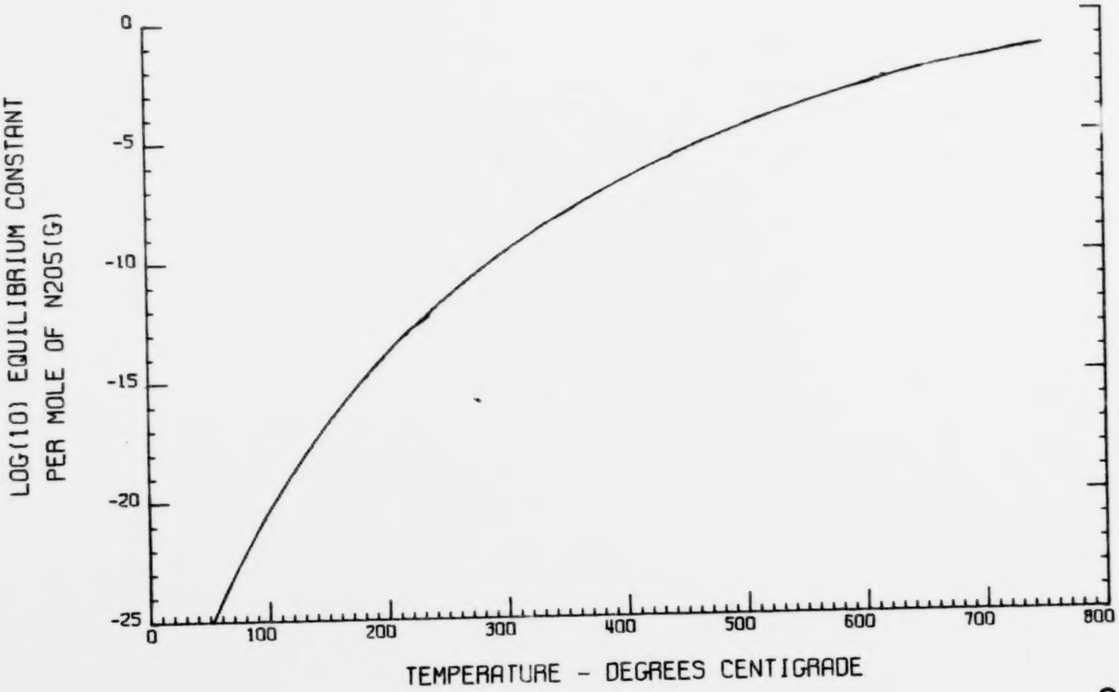
```
11  OCT.  1971                  SR(NO3)2 + CO2 I N2O5(G) + SRCO3

    TEMPERATURE            ENTHALPY              ENTROPY                LOG  K
      DEG. C              CAL./GMOLE        CAL./GMOLE/DEG.K

    2.5000+01             3.9529+04            4.6340+00             -2.7961+01
    5.0000+01             5.3013+04            4.8766+01             -2.5193+01
    1.0000+02             5.2846+04            4.8286+01             -2.0397+01
    1.5000+02             5.2717+04            4.7959+01             -1.6744+01
    2.0000+02             5.2583+04            4.7661+01             -1.3871+01
    2.5000+02             5.2421+04            4.7336+01             -1.1553+01
    3.0000+02             5.2214+04            4.6959+01             -9.6463+00
    3.5000+02             5.1952+04            4.6522+01             -8.0526+00
    4.0000+02             5.1628+04            4.6022+01             -6.7033+00
    4.5000+02             5.1237+04            4.5462+01             -5.5486+00
    5.0000+02             5.0774+04            4.4844+01             -4.5515+00
    5.5000+02             5.0239+04            4.4173+01             -3.6842+00
    6.0000+02             4.9628+04            4.3453+01             -2.9249+00
    6.5000+02             3.8285+04            3.1083+01             -2.2704+00
    7.0000+02             3.7521+04            3.0277+01             -1.8092+00
    7.5000+02             3.6678+04            2.9433+01             -1.4019+00

         HR PLOT COMPLETED
         SR PLOT COMPLETED
         LOG K PLOT COMPLETED
```

SR(NO3)2 + CO2 - N2O5(G) + SRCO3

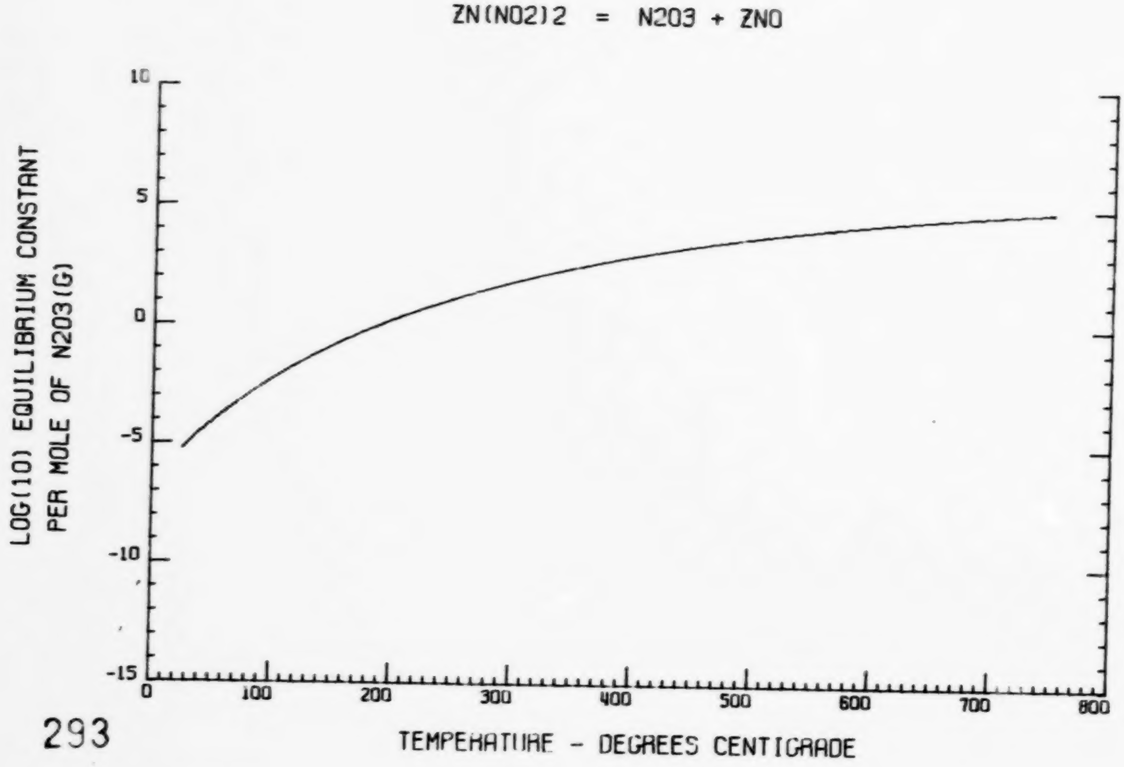


```
9 SEPT.  1971                              ZN(NO2)2  =  N2O3 + ZNO

        TEMPERATURE              ENTHALPY                ENTROPY                  LOG  K
          DEG. C                CAL./GMOLE          CAL./GMOLE/DEG.K

         2.5000+01              2.0004+04              4.3402+01              -5.1770+00
         5.0000+01              2.0028+04              4.3481+01              -4.0421+00
         1.0000+02              2.0092+04              4.3664+01              -2.2245+00
         1.5000+02              2.0134+04              4.3769+01              -8.3258-01
         2.0000+02              2.0122+04              4.3745+01               2.6617-01
         2.5000+02              2.0037+04              4.3576+01               1.1529+00
         3.0000+02              1.9868+04              4.3268+01               1.8804+00
         3.5000+02              1.9604+04              4.2828+01               2.4845+00
         4.0000+02              1.9241+04              4.2269+01               2.9906+00
         4.5000+02              1.8774+04              4.1600+01               3.4178+00
         5.0000+02              1.8199+04              4.0832+01               3.7795+00
         5.5000+02              1.7515+04              3.9975+01               4.0862+00
         6.0000+02              1.6718+04              3.9037+01               4.3467+00
         6.5000+02              1.5809+04              3.8024+01               4.5674+00
         7.0000+02              1.4785+04              3.6945+01               4.7537+00
         7.5000+02              1.3646+04              3.5804+01               4.9099+00

             HR PLOT COMPLETED
             SR PLOT COMPLETED
             LOG K PLOT COMPLETED
```



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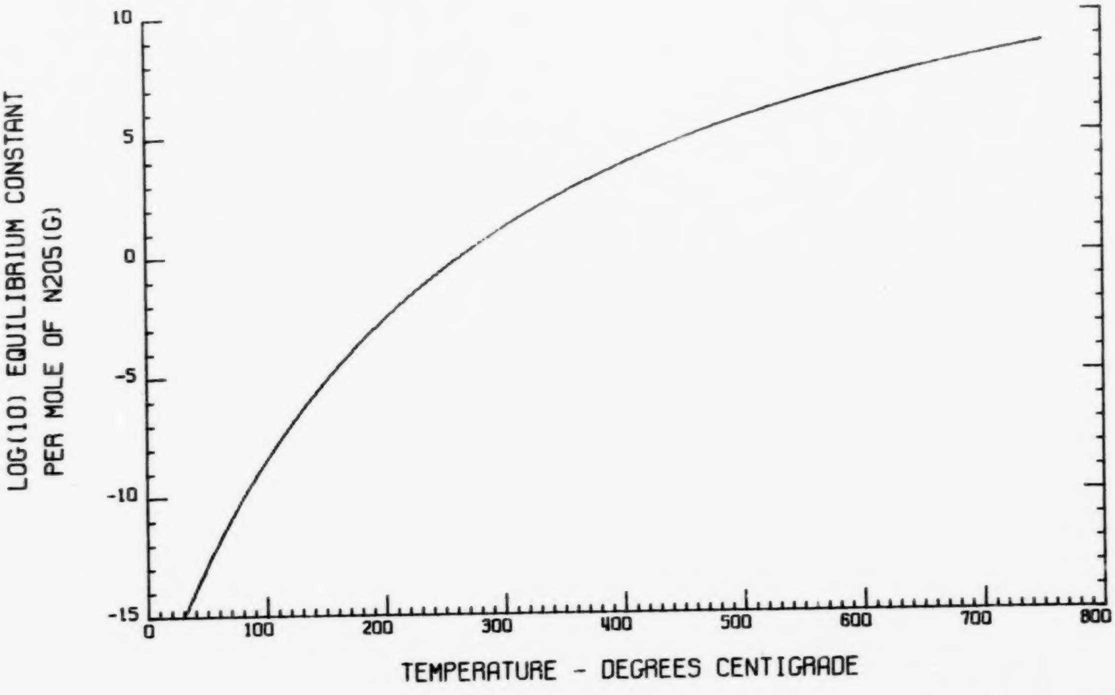
```
9 SEPT.  1971                  ZN(NO3)2  =  N2O5 + ZNO


   TEMPERATURE             ENTHALPY               ENTROPY                LOG  K
    DEG. C               CAL./GMOLE         CAL./GMOLE/DEG.K

   2.5000+01             3.4924+04              4.6992+01              -1.5328+01
   5.0000+01             4.8362+04              9.0981+01              -1.2825+01
   1.0000+02             4.8034+04              9.0035+01              -8.4545+00
   1.5000+02             4.7687+04              8.9165+01              -5.1420+00
   2.0000+02             4.7317+04              8.8337+01              -2.5491+00
   2.5000+02             4.6916+04              8.7534+01              -4.6885-01
   3.0000+02             4.6484+04              8.6745+01               1.2333+00
   3.5000+02             4.6018+04              8.5965+01               2.6486+00
   4.0000+02             4.5516+04              8.5191+01               3.8410+00
   4.5000+02             4.4978+04              8.4420+01               4.8568+00
   5.0000+02             4.4402+04              8.3650+01               5.7304+00
   5.5000+02             4.3788+04              8.2882+01               6.4876+00
   6.0000+02             4.3137+04              8.2113+01               7.1485+00
   6.5000+02             4.2446+04              8.1345+01               7.7287+00
   7.0000+02             4.1717+04              8.0576+01               8.2407+00
   7.5000+02             4.0949+04              7.9806+01               8.6944+00

        HR PLOT COMPLETED
        SR PLOT COMPLETED
        LOG K PLOT COMPLETED
```

ZN(NO3)2 = N2O5 + ZNO



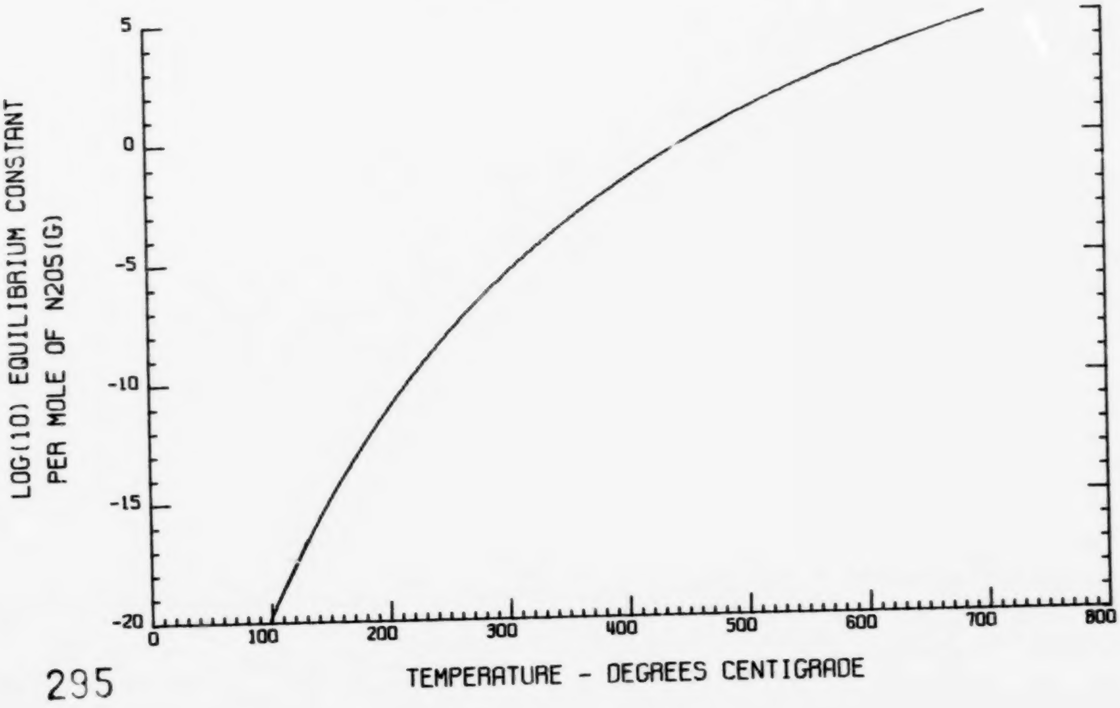
09 SEP 71

```
9 SEPT.  1971                          ZR(NO3)4  =  2N2O5 + ZRO2

                                                                                     LOG  K
                                                       ENTROPY
 TEMPERATURE                 ENTHALPY             CAL./GMOLE/DEG.K
   DEG. C                   CAL./GMOLE
                                                                                 -2.9849+01
                             5.7052+04                5.4761+01                  -2.6089+01
  2.5000+01                  7.0490+04                9.8749+01                  -1.9716+01
  5.0000+01                  7.0161+04                9.7803+01                  -1.4872+01
  1.0000+02                  6.9815+04                9.6933+01                  -1.1072+01
  1.5000+02                  6.9444+04                9.6104+01                  -8.0146+00
  2.0000+02                  6.9044+04                9.5301+01                  -5.5061+00
  2.5000+02                  6.8611+04                9.4512+01                  -3.4140+00
  3.0000+02                  6.8145+04                9.3732+01                  -1.6452+00
  3.5000+02                  6.7643+04                9.2957+01                  -1.3268-01
  4.0000+02                  6.7104+04                9.2186+01                   1.1733+00
  4.5000+02                  6.6528+04                9.1416+01                   2.3104+00
  5.0000+02                  6.5915+04                9.0647+01                   3.3077+00
  5.5000+02                  6.5263+04                8.9879+01                   4.1879+00
  6.0000+02                  6.4572+04                8.9110+01                   4.9689+00
  6.5000+02                  6.3843+04                8.8341+01                   5.6654+00
  7.0000+02                  6.3074+04                8.7571+01
  7.5000+02

        HR PLOT COMPLETED
        SR PLOT COMPLETED
        LOG K PLOT COMPLETED
```

ZR(NO3)4 = 2N205 + ZR02



09 SEP 71

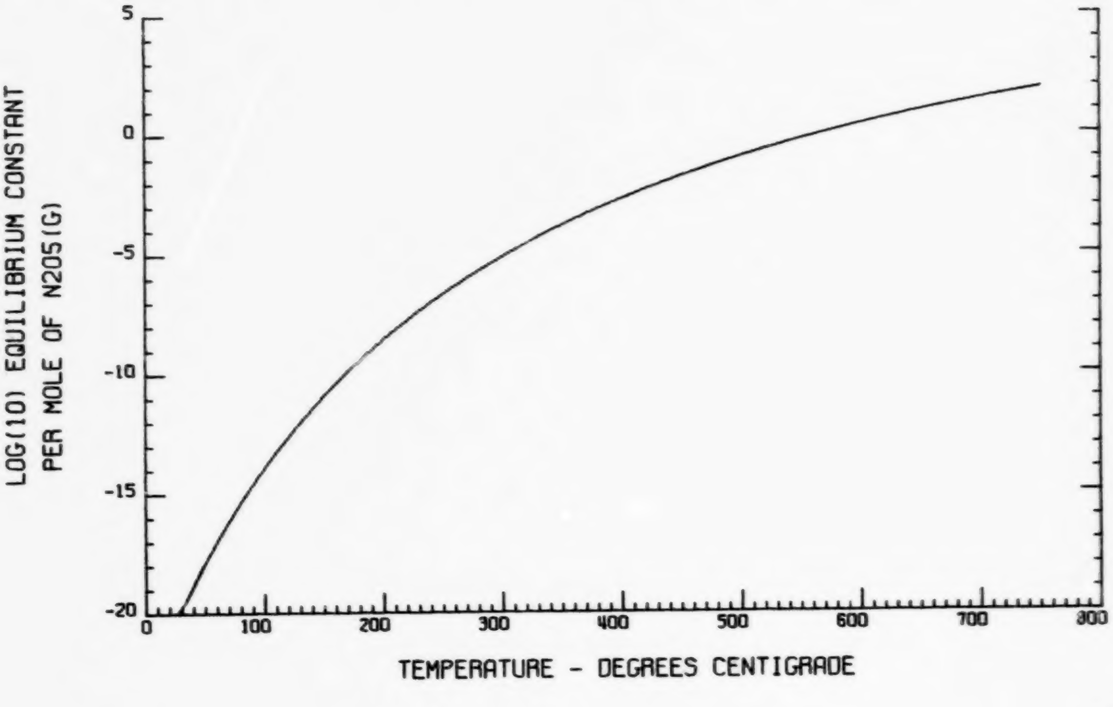
```
11  OCT.  1971                ZR(NO3)4 + 2CO2 I  2N2O5 + ZR(CO3)2

    TEMPERATURE              ENTHALPY              ENTROPY              LOG  K
     DEG. C                 CAL./GMOLE        CAL./GMOLE/DEG.K

    2.5000+01               3.0435+04             1.0161+01           -2.0087+01
    5.0000+01               4.3866+04             5.4126+01           -1.7836+01
    1.0000+02               4.3581+04             5.3303+01           -1.3874+01
    1.5000+02               4.3331+04             5.2675+01           -1.0867+01
    2.0000+02               4.3093+04             5.2143+01           -8.5081+00
    2.5000+02               4.2851+04             5.1658+01           -6.6110+00
    3.0000+02               4.2597+04             5.1193+01           -5.0539+00
    3.5000+02               4.2323+04             5.0735+01           -3.7547+00
    4.0000+02               4.2025+04             5.0276+01           -2.6560+00
    4.5000+02               4.1702+04             4.9813+01           -1.7162+00
    5.0000+02               4.1350+04             4.9343+01           -9.0452-01
    5.5000+02               4.0969+04             4.8865+01           -1.9774-01
    6.0000+02               4.0557+04             4.8380+01            4.2207-01
    6.5000+02               4.0115+04             4.7887+01            9.6896-01
    7.0000+02               3.9641+04             4.7388+01            1.4541+00
    7.5000+02               3.9136+04             4.6882+01            1.8864+00

         HR PLOT COMPLETED
         SR PLOT COMPLETED
         LOG K PLOT COMPLETED
```

ZR(NO3)4 + 2CO2 → 2N2O5 + ZR(CO3)2



Radian Corporation

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TECHNICAL NOTE 200-007-16

LISTING OF SUBROUTINES FOR THE GAS PHASE EQUILIBRIUM MODEL

13 January 1972

Prepared by:

Terry B. Parsons

T. I. Strange

CHEMICAL RESEARCH • SYSTEMS ANALYSIS • COMPUTER SCIENCE • CHEMICAL ENGINEERING

The following pages are listings of the subroutines GASEQS, INIT, GPEQS, GPARTL, and GTEMP. These subroutines were written to calculate the concentrations of NO, NO_2, N_2O_3, N_2O_4, N_2O_5, H_2O, HNO_2 and HNO_3 present at equilibrium under specified conditions of total pressure, temperature, and number of moles of chemical NO, NO_2, and H_2O. The detailed problem definition and a description of the method of solution are given in Technical Note 200-007-03a.

GASEQS calls the subroutine NOLIN which calls some additional subroutines. NOLIN and the additional subroutines needed for using the gas phase equilibrium model have already been published in a Radian report entitled "A Theoretical Description of the Limestone Injection - Wet Scrubbing Process." Volume II, Final Report to NAPCA, Contract No. CPA-22-69-138 9 June 1970. The report is available through the National Technical Information Service, Operations Division, U. S. Department of Commerce, Springfield, Virginia, 22151. The order number is PB 193-030.

Subroutine INIT

```
@I FOR INIT
      SUBROUTINE INIT(X,CM,P)
      COMMON/FUNC/F(50),CK(50),CT(10)
      DIMENSION X(1),CM(1)
C
      DEFINE GTEMP(I)=EXP(CK(I))
C
      IF(CM(1).LE.0.0) GOTO 2
      ESTMOL = CM(1)+CM(3)+X(1)
      X(2) = CM(1)/ESTMOL                                                    NO
      X(3) = CM(2)/ESTMOL                                                    NO2
      X(10)=1./P*(X(3)/(GTEMP(6)*X(2)))**2
    4 CONTINUE
      X(4) = X(2)*X(3)*P*GTEMP(2)                                            N2O3
      X(5) = X(3)*X(3)*P*GTEMP(1)                                            N2O4
      X(6) = CM(3)/ESTMOL                                                    H2O
      X(7) = SQRT(X(4)*X(6)*GTEMP(4))                                        HNO2
      X(8) = X(5)*X(6)*GTEMP(3)/X(7)                                         HNO3
      X(9) = X(5)*X(3)/GTEMP(5)/X(2)                                         N2O5
      DO 1 I=2,10
      IF(X(I).LE.0.) X(I)=1.E-37
    1 CONTINUE
      RETURN
    2 CONTINUE
      RAT=CM(2)/CM(1)
      IF(RAT.GT.-3.0) GOTO 3
      X(3)=(CM(2)+CM(1))/ESTMOL
      X(10)=-CM(1)/(2.0*ESTMOL)
      X(2)=SQRT(P*X(10))/X(3)/GTEMP(6)
      GOTO 4
    3 CONTINUE
      PRINT 100,RAT
  100 FORMAT(//5X,'RATIO OF CNO2 TO CNO GREATER THAN -3.0 WHICH IS PHYSI
     *CALLY IMPOSSIBLE, RATIO = ',E10.4//)
      CALL EXIT
      RETURN
      END
```

Subroutine GPEQS

```
@I FOR GPEQS
      SUBROUTINE GPEQS(W)
      COMMON /FUNC/ F(50),CK(50),CT(10)
      COMMON /GAS/ PLN,FUCF(50),TH(10)
      COMMON/LIMS/NF,NL
      DIMENSION W(1),X(50),EQ(50)
      DOUBLE PRECISION F,CK,CT,W,X,EQ,PLN,FUCF,TH
C
      DEFINE Y(I)=EXP(X(I))
C
      DO 1 I=1,NF
      J=I+1
      X(J)=W(I)
    1 CONTINUE
      IF(NF.EQ.8) X(10)=-88.
      IF(X(10).GT.0.0) X(10)=0.0
C
      EQ(1)=CK(1)+PLN+2*FUCF(3)-FUCF(5)+2*X(3)-X(5)
      EQ(2)=CK(2)+PLN+FUCF(2)+FUCF(3)-FUCF(4)+X(2)+X(3)-X(4)
      EQ(3)=CK(3)+FUCF(5)+FUCF(6)-FUCF(7)-FUCF(8)+X(5)+X(6)-X(7)-X(8)
      EQ(4)=CK(4)+FUCF(4)+FUCF(6)-2*FUCF(7)+X(4)+X(6)-2*X(7)
      EQ(8)=CK(5)+FUCF(2)+FUCF(9)-FUCF(5)-FUCF(3)+X(2)+X(9)-X(5)-X(3)
      EQ( 9)=CK(6)+FUCF(2)+.5*FUCF(10)-FUCF(3)+X(2)+.5*X(10)-X(3)+.5*PLN
      TH(1)=Y(4)+Y(5)+.5*Y(7)+.5*Y(8)+1.+Y(9)-Y(10)
      TH(2)=Y(3)+2*Y(5)+Y(4)+.5*Y(7)+1.5*Y(8)+3*Y(9)+.5*Y(10)
      EQ(5)=CT(1)+LOG(TH(1))-LOG(TH(2))
      TH(3)=Y(2)+Y(3)+2*Y(4)+2*Y(5)+Y(7)+Y(8)+2*Y(9)
      EQ(6)=CT(2)+LOG(TH(1))-LOG(TH(3))
      TH(4)=Y(3)+2*Y(5)+Y(4)+Y(6)+Y(7)+2*Y(8)+3*Y(9)+.5*Y(10)
      EQ(7)=CT(3)+LOG(TH(1))-LOG(TH(4))
C
      DO 2 I=1,NF
      F(I)=EQ(I)
    2 CONTINUE
      RETURN
      END
```

Subroutine GASEQS

```
@I FOR GASEQS
      SUBROUTINE GASEQS(X,CM,P,TK,IOPT)
      COMMON /FUNC/F(50),CK(50),CT(10)
      COMMON /GAS/PLN,FUCF(50),TH(10)
      COMMON/LIMS/NF,NL
      EXTERNAL GPEQS,GPARTL
      DIMENSION X(1),CM(1),LB(60),
     *XLN(50)
      DOUBLE PRECISION F,CK,CT,PLN,FUCF,TH,XLN
      DATA (LB(I),I=1,9)/'INERTS','NO    ','NO2   ','N203  ','N204  ',
     *'H20   ','HNO2  ','HNO3  ','N205  '/
      DATA LB(10)/'02    '/
      DATA FUCF/50*0./
C
      NF=8
      IF(IOPT.NE.0) NF=9
      EPS=1.E-4
C
      CALL GTEMP(TK)
C
      CALL INIT(X,CM,P)
      PLN=LOG(P)
      SCJ=CM(1)+CM(2)+CM(3)
      CT(1)=LOG(CM(2)/(X(1)+SCJ))
      CT(2)=LOG((CM(1)+CM(2))/(X(1)+SCJ))
      CT(3)=LOG((CM(2)+CM(3))/(X(1)+SCJ))
C
      NM=NF-1
      NL=NF+1
      DO 1 I=1,NM
      J=I+1
      XLN(I)=LOG(X(J))
    1 CONTINUE
      WRITE(6,100)
      CALL DATIME
      TC=TK-273.16
      WRITE(6,107) TC
      WRITE(6,103)
      WRITE(6,104) (CM(I),I=1,3),P
      WRITE(6,105)
      WRITE(6,106)
  100 FORMAT(1H1)
  101 FORMAT(15X,A6,6X,1PE12.5,5X,1PE12.5,7X,1PE12.5,7X,1PE12.5)
  102 FORMAT(//5X,'TOTAL MOLES = ',1PE12.5,20X,'RESIDUAL ERROR =',1PE12.
     *5)
  103 FORMAT(42X,'INPUT MOLES'/)
  104 FORMAT(10X,'NO = ',1PE11.5,5X,'NO2 = ',1PE11.5,5X,'H20 = ',1PE11.5
     *,5X,'PRESSURE = ',1PE11.5,' ATM.'///)
  105 FORMAT(40X,'GAS PHASE EQUILIBRIA'//)
  106 FORMAT(48X,  'MOLE',T67,'PARTIAL',T86,'FUGACITY'/15X,'COMPONENT',
     *              T32,'MOLES',T48,'FRACTION',T67,'PRESSURE',T86,'COEFFIEN
     *T'/)
  107 FORMAT(1H+,70X,'TEMPERATURE',F10.3,' DEG C.')
  108 FORMAT(27X,'NORMALIZED MATERIAL BALANCE ERROR =',1PE12.5)
C
      CALL NOLIN(XLN,NF,EPS,GPEQS,GPARTL)
C
      DO 2 I=2,NL
      J=I-1
      X(I)=EXP(XLN(J))
    2 CONTINUE
      TM=(X(1)+SCJ)/(1.+X(4)+X(5)+.5*X(7)+.5*X(8)+X(9)-X(10))
C
      FU=EXP(FUCF(1))
      FM=X(1)/TM
      PP=FM*P
      WRITE(6,101) LB(1),X(1),FM,PP,FU
C
C
      DO 5 I=2,NL
      XM=X(I)*TM
      PP=X(I)*P
      FU=EXP(FUCF(I))
      WRITE(6,101) LB(I),XM,X(I),PP,FU
    5 CONTINUE
      SUM=0.
      DO 4 I=1,NF
      SUM=SUM+F(I)*F(I)
    4 CONTINUE
      RE=SUM
      WRITE(6,102) TM,RE
      SUM=FM
      DO 3 I=2,NL
      SUM=SUM+X(I)
    3 CONTINUE
      EMB=(CM(1)+CM(2)-TM*(X(2)+X(3)+2.*X(4)+2.*X(5)+X(7)+X(8)+2.*X(9)))
     */(CM(1)+CM(2))
      WRITE(6,108) EMB
      RETURN
      END
```

Subroutine GPARTL

```
@I FOR GPARTL
      SUBROUTINE GPARTL(W)
      COMMON /FUNC/F(50),CK(50),CT(10)
      COMMON/GRAD/PD(50,50),AS(50,50),SQ(50)
      COMMON /GAS/PLN,FUCF(50),TH(10)
      COMMON/LIMS/NF,NL
      DIMENSION W(1),X(50),GD(50,50)
      DOUBLE PRECISION F,CK,CT,PD,AS,SQ,PLN,FUCF,TH,W,X,GD,BR
C
      DEFINE Y(I)=EXP(X(I))
C
      IF(NF.EQ.8) X(10)=-88.
      DO 1 I=1,NF
      DO 2 J=1,NF
      GD(I,J)=0.
    2 CONTINUE
      J=I+1
      X(J)=W(I)
    1 CONTINUE
C
      GD(1,3)=-2.
      GD(1,5)= 1.
      GD(2,2)=-1.
      GD(2,3)=-1.
      GD(2,4)= 1.
      GD(3,5)=-1.
      GD(3,6)=-1.
      GD(3,7)= 1.
      GD(3,8)= 1.
      GD(4,4)=-1.
      GD(4,6)=-1.
      GD(4,7)= 2.
      GD(8,2)=-1.
      GD(8,9)=-1.
      GD(8,5)= 1.
      GD(8,3)= 1.
      GD( 9,10)=-.5
      GD( 9,3)=+1.
      GD( 9,2)=-1.
C


      BR=TH(1)
      DO 3 I=5,7
      GD(I,4)=-Y(4)/BR
      GD(I,5)=-Y(5)/BR
      GD(I,7)=-.5*Y(7)/BR
      GD(I,8)=-.5*Y(8)/BR
      GD(I,10)=Y(10)/BR
      GD(I,9)=-Y(9)/BR
    3 CONTINUE
      BR=TH(2)
      GD(5,3)=Y(3)/BR
      GD(5,4)=GD(5,4)+Y(4)/BR
      GD(5,5)=GD(5,5)+2.*Y(5)/BR
      GD(5,7)=GD(5,7)+.5*Y(7)/BR
      GD(5,8)=GD(5,8)+1.5*Y(8)/BR
      GD(5,9)=GD(5,9)+3*Y(9)/BR

      GD(5,10)=GD(5,10)+.5*Y(10./BR
      BR=TH(3)
      GD(6,2)=Y(2)/BR
      GD(6,3)=Y(3)/BR
      GD(6,4)=GD(6,4)+2.*Y(4)/BR
      GD(6,5)=GD(6,5)+2.*Y(5)/BR
      GD(6,7)=GD(6,7)+Y(7)/BR
      GD(6,8)=GD(6,8)+Y(8)/BR
      GD(6,9)=GD(6,9)+2*Y(9)/BR
      BR=TH(4)
      GD(7,3)=Y(3)/BR
      GD(7,4)=GD(7,4)+Y(4)/BR
      GD(7,5)=GD(7,5)+2.*Y(5)/BR
      GD(7,6)=Y(6)/BR
      GD(7,7)=GD(7,7)+Y(7)/BR
      GD(7,8)=GD(7,8)+2.*Y(8)/BR
      GD(7,9)=GD(7,9)+3*Y(9)/BR
      GD(7,10)=GD(7,10)+.5*Y(10)/BR
C
      DO 4 I=1,NF
      DO 5 J=1,NF
      K=J+1
      PD(I,J)=GD(I,K)
    5 CONTINUE
    4 CONTINUE
      RETURN
      END
```

Subroutine GTEMP

```
@I FOR GTEMP
      SUBROUTINE GTEMP(TK)
      COMMON/FUNC/F(50),CK(50),CT(10)
      DOUBLE PRECISION F,CK,CT
      DIMENSION A(10),B(10),C(10),D(10),E(10),G(10)
      DIMENSION LB(6,4),EK(6)
      DATA (LB(1,J),J=1,4)/24H         2*NO2=N2O4      /
      DATA (LB(2,J),J=1,4)/24H        NO+NO2=N2O3      /
      DATA (LB(3,J),J=1,4)/24H      N2O4+H2O=HNO2+HNO3/
      DATA (LB(4,J),J=1,4)/24H      N2O3+H2O=2*HNO2    /
      DATA (LB(5,J),J=1,4)/24H       NO+N2O5=N2O4+NO2 /
      DATA (LB(6,J),J=1,4)/24H     NO+1/2*O2=NO2       /
      DATA(EK(I),I=1,6)/6.82056,.507022,5.73284E-3,.644635,5.24517E9,
     *1.51920E+6/
      DATA (A(I),I=1,6)/-81.527,-56.918,66.013,4.709,31.199,-18.122/
      DATA (B(I),I=1,6)/5.57,3.21,-8.9,-.78,-4.92,-.035/
      DATA (C(I),I=1,6)/-2.365E5,-1.695E5,2.373E5,-.29E5,1.99E5,-.735E5/
      DATA (D(I),I=1,5)/16.837E3,11.724E3,-8.661E3,-.2839E3,1.15138E4/
      DATA D(6)/1.41382E4/
      DATA (E(I),I=1,5)/-6.8E-4,-4.55E-4,27.25E-4,4.5E-4,.001525/
      DATA E(6)/4.5E-5/
      DATA (G(I),I=1,6)/0.,0., 7.667E-8, 7.667E-8,0.,3.0E-8/
      IF(TOLD.EQ.TK) RETURN
      R=1.98726
      TKS=TK*TK
      WRITE(6,101)
      TC=TK-273.16
      WRITE(6,102) TC
      WRITE(6,103)
      WRITE(6,104)
  100 FORMAT(20X,4A6,2(5X,1PE12.5)/)
  101 FORMAT(1H1)
  102 FORMAT(41X,'TEMPERATURE ',F10.3,' DEG. C'/)
  103 FORMAT(45X,'EQUILIBRIUM CONSTANTS'/)
  104 FORMAT(31X,  'REACTION',T53,'K(TEMP.)',T70,'K(25 C.)'/)
      DO 1 I=1,6
      CK(I)=(A(I)+B(I)*LOG(TK)+C(I)/TKS  +D(I)/TK +E(I)*TK+G(I)*TKS)/R
      X=EXP(CK(I))
      WRITE(6,100) (LB(I,J),J=1,4),X,EK(I)
    1 CONTINUE
      TOLD=TK
      RETURN
      END
```